Non-linear Anisotropic Mechanical Behaviour of Soft and Hard Tissues

David R. Nolan B.E. (2011)

A thesis submitted to the National University of Ireland as fulfilment of the requirements for the Degree of Doctor of Philosophy

September 2015

Discipline of Biomedical Engineering,
College of Engineering and Informatics,
National University of Ireland, Galway

Supervisor of Research: Dr. J. Patrick McGarry

Head of Discipline: Prof. Peter E. McHugh
To Sarah, for her eternal love and support

To Felix, Emily and Emma for the same, and for making me the person I am today
The overall objective of this thesis is to develop accurate and rigorous constitutive formulations for the non-linear anisotropic behaviour of soft tissue (arterial) and hard tissues (trabecular bone) at large strains.

The Holzapfel–Gasser–Ogden (HGO) constitutive model for anisotropic hyperelastic behaviour of collagen fibre reinforced materials was initially developed to describe the elastic properties of arterial tissue, but is now used extensively for modelling a variety of soft biological tissues. A compressible form (HGO-C model) is widely used in finite element (FE) simulations. Here, by using three simple deformations (pure dilatation, pure shear and uniaxial stretch), it is demonstrated that the compressible HGO-C formulation does not correctly model compressible anisotropic material behaviour, because the anisotropic component of the model is insensitive to volumetric deformation due to the use of isochoric anisotropic invariants. In order to correctly model compressible anisotropic behaviour a modified anisotropic (MA) model is presented, whereby the full anisotropic invariants are used, so that a volumetric anisotropic contributions are accounted for. The MA model correctly predicts an anisotropic response to hydrostatic tensile loading, whereby a sphere deforms into an ellipsoid. It also computes the correct anisotropic stress state for pure shear and uniaxial deformation. To look at more practical applications, a FE user-defined material subroutine is developed and used for the simulation of stent deployment in a slightly compressible artery. Significantly higher stress triaxiality and arterial compliance are computed when the full anisotropic invariants are used (MA model) instead of the isochoric form (HGO-C model).

Biaxial tests are commonly used to investigate the mechanical behaviour of soft biological tissues and polymers. In the current paper a fundamental problem associated with the calculation of material stress from measured force in standard biaxial tests is uncovered. In addition to measured forces, localized unmeasured shear forces also occur at the clamps and the inability to quantify such forces has significant implications for the calculation of material stress from simplified force-equilibrium relationships. Unmeasured shear forces are shown to arise due to two distinct competing contributions: (1) negative shear force due to stretching of the orthogonal clamp, and (2) positive shear force as a result of material Poisson-effect. The clamp shear force is highly dependent on the specimen geometry and the clamp displacement ratio, as consequently, is the measured force-stress relationship. Additionally, it is demonstrated that commonly accepted formulae for the estimation of material stress in the central region of a cruciform specimen are highly inaccurate, and an empirical correction factor for the general case of isotropic materials is established. Finally we demonstrate that a correction factor for the general case of non-linear anisotropic materials is not feasible and we suggest the use of inverse FE analysis as a practical means of interpreting experimental data for such complex materials.

Arterial tissue is commonly assumed to be incompressible. While this assump-
tion is convenient for both experimentalists and theorists, the compressibility of arterial tissue has not been rigorously investigated. The current study presents an experimental-computational methodology to determine the compressibility of aortic tissue and it is demonstrated that specimens excised from an ovine descending aorta are significantly compressible. Specimens are stretched in the radial direction in order to fully characterise the mechanical behaviour of the tissue ground matrix. Additionally, biaxial testing is performed to fully characterise the anisotropic contribution of reinforcing fibres. An inverse FE analysis scheme is implemented to characterise the mechanical behaviour of the arterial tissue. Results reveal that ovine aortic tissue is highly compressible; an effective Poisson’s ratio of 0.44 is determined for the ground matrix component of the tissue. It is also shown that correct characterisation of material compressibility has important implications for the calibration of anisotropic fibre properties using biaxial tests. Finally it is demonstrated that correct treatment of material compressibility has significant implications for the accurate prediction of the stress state in an artery under in vivo type loading.

The inelastic behaviour of trabecular bone is investigated using both mechanical testing and microstructural FE models. Continuum level constitutive models are used to capture the inelastic mechanical behaviour observed in the above in vitro and in silico tests. A series of torsion tests on cylindrical specimens of trabecular bone are performed to determine its inelastic mechanical behaviour under shear loading, these are supplemented by the uniaxial and confined compression experimental data from a previous study. An isotropic Crushable-Foam plasticity model with isotropic hardening (CFIH) is used to model the inelastic experimental data, however it is unable to predict the behaviour over the full range of multiaxial loading tests. A novel hardening function is formulated in which the hardening rate is a function of the deviatoric and volumetric plastic strain (CFMD). This function can more accurately predict the multiaxial post-yield behaviour. Next, micro-structural FE models are used to repeatably test an 8 mm cube of trabecular bone in uniaxial compression, confined compression, and simple shear. An anisotropic pressure-dependent yield function with uniform hardening (XH04) is introduced to model the anisotropic inelasticity of the tissue. The XH04 model fails to predict the mode-dependent hardening observed in the micro-FE tests. A non-uniform hardening model which uses plastic-data functions to determine evolution of the yield function (XH05) is used to model the inelastic behaviour. It is demonstrated that a coupled hardening XH05 model generates significant strain hardening and gives the best prediction of multiaxial behaviour. Finally, it is shown that the inclusion of finite deformations results in a further improvement in the prediction of multiaxial inelastic behaviour.
Acknowledgements

First and foremost I would like to acknowledge the help, support and guidance of my PhD supervisor Dr. Patrick McGarry. All that I have learnt about mechanics in the past four years is as a result of your expertise and enthusiasm for the topic. I aim to uphold the scientific principles you have imparted upon me in my future endeavours.

I would like to thank the academic staff in the departments of Mechanical and Biomedical Engineering for creating an superb environment in which to learn and conduct research. I owe a huge debt of gratitude to the technical staff in the College of Engineering and Informatics, in particular to Pat Kelly and Bony Kennedy for fabricating experimental rigs, and to William Kelly, David Connolly and Maja Drapiewska for assistance in the biomedical lab. A special thanks too to Jane Bowman and Sharon Gilmartin who have always looked after me over the past 8 years. All of the gents in Brady’s Athenry.

I would like thank Prof. Tony Keaveny and Prof. Oliver O’Reilly for facilitating the semester I spent at UC Berkeley.

Thanks too to Prof. Michel Destrade and Prof. Ray Ogden, I was introduced to hyperelasticity by two of its finest practitioners. I also spent some enlightening times at a whiteboard with Dr. Artur Gower, deciphering the “true” meaning of DDSDDE.

I would not have made it though the past four years without my academic soulmate, desk-neighbour and BFF, Noel Reynolds. You’ve always been there for advice and support when things go lemon-shaped. A big thanks too to Lizanne, you complete the circle. I’ve had the good fortune to share the past four years with some exceptionally talented and interesting people. A big thanks to Anna, Brian, Catherine, Caomhe, Claire, Conor, Conleth, Donnacha, Eamonn, Ed, Enda, Emer, Eimear, Eoin, Eoghan, Ewa, Evelyn, Feizhu, Fiona, G,F,W, Heather, Irene, James, Myles, Matt, Mary, Muriel, Niall, Nicola, Orla, Paul, G,W, Reyhanneh, Riona, Sinead, Stefaan, Tarek, Ted, the American Toms, Wejdan, and Will for making work a lot of fun.

I would like to acknowledge the Irish Research Council, Science Foundation Ireland, the College of Engineering and Informatics NUIG, and the UC Education Abroad Program for funding this research. Also the Irish Centre for High-End Computing (ICHEC) for the provision of computational facilities and support.

I would like to thank my parents, Emily and Felix, for their constant love, support and generosity. I’m finish college now! Kinda. A big thanks too to my sister Emma for always sending me messages of support at those critical times.

Finally, but by no means the least, I would like to acknowledge the infinite love, patience and support of my love Sarah McCartan. I would not have been able to do this without you.
List of Publications

First-author journal publications


Publications not included in this thesis


International Conference Proceedings


Greece


Prizes

Engineers Ireland Biomedical Research Medal (2015). This medal is awarded annually by Engineers Ireland at the annual Bioengineering in Ireland conference to a PhD student deemed to be making the most significant contribution to the field of biomedical engineering research in Ireland.
Contents

Abstract i

Acknowledgements iv

List of Publications, Conference Proceedings and Prizes v

1 Introduction and Background to the Literature 1
   1.1 Introduction to the Thesis and Thesis Structure . . . . . . . . . . . . 1
   1.1.1 Objectives . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 2
   1.1.2 Thesis Structure . . . . . . . . . . . . . . . . . . . . . . . . . 3
   1.2 Background and Literature . . . . . . . . . . . . . . . . . . . . . . 6
       1.2.1 Biomechanics of Soft Tissue . . . . . . . . . . . . . . . . . . 6
       1.2.2 Biomechanics of Hard Tissue . . . . . . . . . . . . . . . . . . 23
   Bibliography . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 36

2 Theory 45
   2.1 Continuum Mechanics . . . . . . . . . . . . . . . . . . . . . . . . . 45
       2.1.1 Deformation and Motion . . . . . . . . . . . . . . . . . . . . . 46
       2.1.2 Strain Measures . . . . . . . . . . . . . . . . . . . . . . . . . 49
       2.1.3 Stress . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 60
   2.2 Finite Element Method . . . . . . . . . . . . . . . . . . . . . . . . 63
       2.2.1 Lagrangian Finite Element Equations . . . . . . . . . . . . . . 63
       2.2.2 Solution of the Non-Linear Finite Element Equations . . . . . 65
       2.2.3 Finite Element Discretization . . . . . . . . . . . . . . . . . . 71
       2.2.4 Newton-Raphson Method in Multiple Variables . . . . . . . . 75

vii
2.2.5 Explicit Solution of the Finite Element Equations .......... 75
2.3 Constitutive Laws ........................................... 77
  2.3.1 Linear Elasticity ....................................... 77
  2.3.2 Hyperelasticity ......................................... 78
  2.3.3 The Consistent Tangent Matrix ......................... 87

3 A robust anisotropic hyperelastic formulation for the modelling of soft tissue ................................................. 91
  3.1 Introduction .................................................. 92
  3.2 Theory: Compressible Anisotropic Hyperelastic Constitutive Models ........................................... 95
    3.2.1 HGO-C Model for Compressible Materials ............... 95
    3.2.2 Pure dilatational deformation ........................... 99
    3.2.3 Applied hydrostatic stress .............................. 100
    3.2.4 Modified Anisotropic Model for Compressible Materials . 102
  3.3 Analysis of Pure Shear ...................................... 104
    3.3.1 Plane strain pure shear .................................. 105
    3.3.2 Plane stress pure shear .................................. 107
  3.4 Uniaxial stretch ............................................. 110
  3.5 Finite Element analysis of realistic arterial deformation .......... 111
    3.5.1 Pressure expansion of an artery ......................... 112
    3.5.2 Stent deployment in an artery .......................... 115
  3.6 Concluding remarks .......................................... 117
  3.7 Appendices .................................................. 121

Bibliography ....................................................... 124

4 On the correct interpretation of measured force and calculation of material stress in biaxial tests ................................................. 127
  4.1 Introduction .................................................. 128
  4.2 Methods: Finite element model implementation ................ 130
  4.3 Can standard biaxial force measurement be directly related to material stress? ......................... 133
  4.4 Inaccuracy of standard methods for biaxial stress calculation .......... 142
  4.5 Can simple correction factors be established to improve the accuracy of current standard methods of stress estimation? ......................... 146
  4.6 Concluding remarks .......................................... 151
  4.7 Appendices .................................................. 154
## Bibliography

5 Compressibility of Arterial Tissue and Consequences for Modelling Soft Tissues 165

5.1 Introduction 166

5.2 Materials and Methods 168

5.2.1 Compressible Anisotropic Constitutive Model 168

5.2.2 Compressibility of Arterial Tissue 170

5.2.3 Biaxial Experiments 174

5.3 Results 179

5.3.1 Compressibility of Arterial Tissue and Isotropic Ground Matrix Calibration 179

5.3.2 Confined Compression Test Results 180

5.3.3 Anisotropic Material Constant Calibration 182

5.3.4 Assessment of Error Generated by the Incompressibility Assumption 184

5.4 Discussion 187

5.5 Conclusion 191

5.6 Appendices 192

Bibliography 198

6 Non-uniform hardening plasticity models for the mechanical behaviour of trabecular bone 202

6.1 Introduction 203

6.2 Theoretical Framework 206

6.2.1 Fundamental equations 206

6.2.2 Finite deformation plasticity 209

6.3 Numerical Implementation 215

6.3.1 Predictor-corrector algorithm 215

6.3.2 Finite deformation implicit stress update algorithm 217

6.3.3 Numerical Consistent Tangent Matrix 222

6.4 Mode-Dependent Strain Hardening 226

6.4.1 Multiaxial mechanical tests on trabecular bone 226

6.4.2 Prediction of multiaxial stress-strain behaviour using a Crushable-Foam model 227

6.4.3 Formulation of a new hardening function 232
6.5 Anisotropic Plasticity .................................................. 239
  6.5.1 Micro-mechanical finite element analysis .................... 239
  6.5.2 Anisotropic yield surfaces and hardening functions ....... 243
6.6 Discussion ............................................................... 260
Bibliography ............................................................... 264

7 Concluding Remarks .................................................... 269
  7.1 Summary of Key Findings ............................................ 269
  7.2 Future Perspectives .................................................. 272
Bibliography ............................................................... 275

A Abaqus User Subroutines .............................................. 277
  A.1 uanisohyper_inv ...................................................... 277
    A.1.1 Derivatives of the Modified Anisotropic Hyperelastic Constitutive Law .................................................. 277
    A.1.2 MATLAB Code to Compute Strain Energy Derivatives ...... 279
Declaration of Originality

I certify that the work presented in this thesis is my own

    David Nolan
Introduction and Background to the Literature

1.1 Introduction to the Thesis and Thesis Structure

The structure and mechanical behaviour of soft biological tissue is extremely complex. In the case of arterial tissue, collagen fibres are helically arranged around the circumference of the vessel wall Humphrey (2002). In the case of cartilage, collagen fibre alignment changes with increasing surface depth, from horizontal alignment in the superficial zone to vertical alignment in the deep zone (Jeffery et al., 1991). Despite this structural complexity, several studies use over-simplified models (Carew et al., 1968; Lai et al., 1991; Karimi et al., 2014; Perktold and Rappitsch, 1995),

But to make an enemy of Newton was fatal.
For Newton, right or wrong, was implacable.

Margaret 'Espinasse on Isaac Newton’s rivalry with Robert Hooke
neglecting material non-linearity and anisotropy. Additionally a number of studies incorrectly implement compressible behaviour of anisotropic soft tissue (Cardoso et al., 2014; Iannaccone et al., 2014).

While aligned collagen fibres are also a key structural feature of hard tissue (bone), it behaves significantly differently to soft tissue due to a high content of mineralized hydroxyapatite (HA) crystals. Bone therefore exhibits a high strength compared to soft tissue and unlike soft tissue, bone exhibits plastic yielding at relatively low strains 0.5–3.5%. Due to its complex open-celled microstructure, trabecular bone can undergo significant permanent volume change, either as a result of medical trauma (Purcell et al., 2013) or device implantation (Kelly et al., 2013). Despite this observation, several studies incorrectly treat the behaviour of trabecular bone using either a pressure-independent von Mises plasticity model, where volume is preserved post-yield (Keyak and Rossi, 2000; Lotz et al., 1991), or friction based plasticity models, in which infinitesimal volume changes inhibit yielding (Bessho et al., 2007; Wang et al., 2008). Such formulations fail to account for the ability of trabecular bone to undergo permanent volumetric deformations/crushing, and also fail to account for anisotropic yielding.

1.1.1 Objectives

The overall objective of this thesis is to develop accurate and rigorous constitutive formulations for the non-linear anisotropic behaviour of soft tissue (arterial) and hard tissues (trabecular bone) at large strains. The specific aims of the current research are given as follows:

1. To develop a robust anisotropic hyperelastic constitutive law for compressible soft tissue.

2. To provide a fundamental analysis of the relationship between measured force
and material stress in biaxial testing of soft tissue.

3. To determine the compressibility of arterial tissue, and quantify its influence on the prediction of artery wall stress.

4. To formulate a constitutive model which can predict the post-yield hardening behaviour of trabecular bone under multiaxial loading conditions.

1.1.2 Thesis Structure

This manuscript is presented for examination under the category of an “Article-Based” thesis. Four journal papers (three published, one under review) form the backbone of the thesis (Chapters 3-6). In accordance with the university guidelines for an “Article-Based” thesis, Chapters 3-6 are reproduced in their published form without alteration to the content. A brief outline of each chapter is given as follows:

Chapter 1: The remaining sections of the current chapter presents a general literature review outlining the foundations of arterial and trabecular bone biomechanics. Key literature concerning constitutive law development and experimental methodologies is presented. In addition to this literature review, a critical and focused analysis of relevant literature is presented in each technical chapter (3-6) in the context of the reported findings of each chapter.

Chapter 2: A background is provided in the theory of continuum mechanics and finite element analysis. Additionally some basic constitutive law development is discussed. The theoretical concepts introduced in this chapter are used for the constitutive law development in technical chapters (3-6).

Chapter 3: (Nolan et al., 2014). A compressible form of the Holzapfel–Gasser–
Ogden (HGO) model is commonly used in finite element analysis software (Abaqus V6.11, 2001; ADINA, 2005). This form uses isochoric anisotropic invariants in its strain-energy density function, which neglects volumetric deformations and leads to the calculation of erroneous stress states. A modified anisotropic (MA) model is proposed which includes stress due to volumetric deformations. It is demonstrated through a number of case studies that this MA model corrects the erroneous behaviour exhibited by the HGO-C model. Finally, a number of simulations of realistic arterial deformations show that use of the modified model leads to the computation of different artery wall stress states than that computed by the compressible HGO-C model.

Chapter 4: Nolan and McGarry (2016). One of the most popular techniques of determining the mechanical properties of anisotropic planar soft tissues is biaxial testing. Here, it is shown that in biaxial tests of cruciform specimens significant shear forces develop at the clamps. Such shear forces are unmeasured by the load cells in a standard experimental setup. The unmeasured shear force makes the calculation of material stress using standard formulae impossible. An analytical model is formulated which uncovers the contribution to this unmeasured shear force, and how it changes as a function of specimen geometry.

Chapter 5: (Nolan and McGarry, 2015a). An experimental study on the compressibility of arterial tissue is performed. Cylindrical specimens of arterial tissue are subjected to a tensile stretch in the radial direction, and volume change is measured using an imaging technique. The tissue is found to be compressible, and its material properties are calculated. Biaxial tests are performed, and the anisotropic material properties determined assuming a) compressibility, and b) incompressibility. The difference in material properties between a) and b) leads to a significant
difference in the stress computed in the vessel wall due to lumen pressure.

**Chapter 6:** (Nolan and McGarry, 2015b). The multiaxial inelastic behaviour of trabecular bone is examined using both experimental testing, and micromechanical finite element models. It is demonstrated that the isotropic Crushable-Foam model with isotropic hardening cannot predict multiaxial yield and hardening behaviour. A new mode-dependent hardening model is introduced, which changes its hardening behaviour depending on the ratio of deviatoric to volumetric deformation. It is demonstrated that this new model leads to improved predictions of multiaxial post-yield behaviour. An anisotropic yield surface is introduced, together with independent and coupled hardening functions. It is demonstrated that the coupled hardening function provides improved predictions of multiaxial hardening behaviour.

**Chapter 7:** Key contributions of the thesis are summarised and recommendations for future work are provided.
1.2 Background and Literature

This thesis is concerned with the anisotropic non-linear behaviour of hard and soft biological tissues at large strains. In this section a general overview of the literature is presented. In Section 1.2.1 previous studies on the mechanical behaviour of soft (arterial) tissues are critiqued. In Section 1.2.2 the mechanical behaviour of hard tissue (trabecular bone) is outlined.

The reader should note that a focused and critical analysis of the relevant literature is provided in each technical chapter (3-6), in the specific context of the key findings of each chapter.

1.2.1 Biomechanics of Soft Tissue

In this section, the literature pertaining the soft tissue mechanics presented in this thesis is presented. First the anatomical structure of the artery is presented. Next, some strain-energy density functions which are used to model the mechanical behaviour of arterial tissue are given. Then, common methodologies for performing and analysing biaxial mechanical tests are presented. Finally, the experimental work which has been performed to date on the compressibility of arterial tissue is reviewed.

1.2.1.1 Structure of Arterial Tissue

The cardiovascular system extends throughout the body. One if its subsystems, the arterial vasculature, is a high pressure conduit through which oxygen-rich blood is transported. The diameter of the artery typically depends on its proximity to the heart, the more distal it is, the smaller the diameter (Fox, 2002). Arteries are divided into two categories: elastic and muscular. Elastic arteries are typically larger in diameter and are more proximal to the heart, while muscular arteries are smaller diameter and more distal (Humphrey, 2002). Some of the most commonly examined
arteries in biomechanics are; the coronary (heart), the carotid (neck), the abdominal (below the diaphragm), and the femoral (upper leg). Figure 1.1 shows a schematic of the artery wall, which is a complex structure consisting of three distinct layers; the intima, the media, and the adventitia (Humphrey, 2002; Marieb and Hoehn, 2007).

The intima is the innermost layer of the artery. It consists of a single layer of endothelial cells resting on a basal membrane, and is similar in both elastic and muscular arteries. In the healthy artery the intima is not considered to contribute to the mechanical strength of the vessel wall, however with increased age the intima thickens and may become mechanically significant (Humphrey, 2002; Klabunde, 2004). Disease of the arteries, known as atherosclerosis, is associated with changes to the intima. Deposition of lipids, calcium, collagen, and fibrin results in the development of an atherosclerotic plaque. These result in structural changes to the artery wall, significantly altering its mechanical properties (Holzapfel et al., 2000; Marieb and Hoehn, 2007).

The middle layer of the artery is known as the media, which consists of smooth muscle cells, elastin and collagen (types I, III and V) fibrils arranged into membranous layers (Marieb and Hoehn, 2007). The direction and orientation of the layers vary with anatomical location, but typically the smooth muscle is aligned in the axial-circumferential plane of the artery wall, forming a helical pattern. The small pitch angle of this helical pattern means that the smooth muscle alignment is close to the circumferential direction. The number of elastic layers decreases peripherally and are hardly present in muscular arteries. The media layer gives the artery high strength in the circumferential and longitudinal directions (Holzapfel et al., 2000; Humphrey, 2002).

The adventitia is the outermost layer of the artery wall and consists of a dense network of type I collagen fibres with admixed elastin, nerves, fibroblasts and vasa
vasorum (Marieb and Hoehn, 2007; Fox, 2002). The collagen fibres in the adventitia are orientated in a more axial direction, reinforcing the strength and stability of the wall. In the event of over-distension, the collagen fibres in the adventitia straighten out and become substantially stiff to counteract this, and prevent rupture (Humphrey, 2002).

1.2.1.2 Strain Energy Functions used for Arterial Tissue

A substantial discussion on the topics of finite deformation kinematics and deformation, and hyperelasticity are presented in Chapter 2. In this thesis arterial tissue is regarded as a mechanically passive material, the main structural components of which are the ground matrix, elastin and collagen fibres. Of course arterial tissue also has an active mechanical response from the activation of smooth muscle cells in the arterial wall.
The majority of constitutive models for arterial tissue are based on the passive response and are based on either a phenomenological or a combined phenomenological-structural approach (Holzapfel et al., 2000; Humphrey, 2002). These models aim to capture the mechanical behaviour at physiological loadings, and take a macro-scale continuum approach to modelling the tissue. This makes it possible\(^1\) to fit the models to experimental data, be they uniaxial, biaxial or lumen inflation tests. As the stress–strain behaviour of arterial tissue is non-linear, various strain energy functions have been formulated using exponential, logarithmic, and polynomial expressions in order to capture this non-linearity. A summary of just some of strain energy density functions which have been formulated for arterial tissue is compiled in Table 1.1.

One of the most popular hyperelastic models for arterial tissue is the Fung model Fung (1967); Fung et al. (1979) which was originally postulated in two dimensions. Several modifications have been added subsequently which generalise the model to include shear deformations and into three dimensions (Sun and Sacks, 2005). There is no physical interpretation for material parameters in the Fung model, consequently it is difficult to place logical bounds for them. One key criterion is that the parameters chosen must ensure convexity of the strain energy density function (Wilber and Walton, 2002).

Several structural constitutive laws have been proposed for arterial tissue. Generally, these models discretise the mechanical behaviour of the tissue into its two primary structural components; its reinforcing fibres and the ground matrix in which they are embedded.

Early work by Tozeren (1984) modelled the mechanical response of the helically wound fibres in the arterial wall, however omitted a ground matrix from the model. Wuyts et al. (1995) assumes that collagen fibrils are embedded circumferentially

\(^1\)As we shall see in the coming chapters, this process is not trivial. Careful consideration must be given to the interpretation of experimental data, and the assumptions which are in-built into constitutive models.
around the arterial wall. The collagen fibrils are assigned a length via a statistical
distribution. Initially a fibril is quite compliant before behaving as a stiff linear
elastic material.

An influential paper outlining the formulation and computational implementa-
tion of structural based models for transversely isotropic biological tissues was
presented by Weiss et al. (1996). This paper is based on constitutive models for
composite materials proposed by Spencer et al. (1984), and suggests the use of an
exponential function of the anisotropic strain invariant, $I_4$, for the strain energy
function.

Holzapfel et al. (2000) proposed such a constitutive model for incompressible
anisotropic arterial tissue. The strain energy density uses two anisotropic strain
invariants, $I_4$ and $I_6$, to prescribe an orthotropic material. A follow-up paper de-
scribes the inclusion of fibre dispersion in a material, using a distribution function
which is a function of a single scalar material parameter, $\kappa$ (Gasser et al., 2006).
These two constitutive models (Holzapfel et al., 2000; Gasser et al., 2006) are the
two most influential in soft tissue biomechanics.
\[ W \]

\begin{align*}
W &= c [\exp(Q(E)) - 1]; \\
Q(E) &= f(E_{ij}, E^2_{ij}, E^3_{ij}, \Lambda)
\end{align*}

Fung (1967)

\[ c_1 E_{\theta\theta}^2 + c_2 E_{\theta\theta} E_{zz} + c_3 E_{zz}^2 + c_4 E_{zz}^3 + c_5 E_{\theta\theta}^2 E_{zz} + c_6 E_{\theta\theta} E^2_{zz} + c_7 E^3_{zz} \]

Vaishnav et al. (1973)

\[ \frac{c}{2} \left[ \exp(a_1 E_{11}^2 + a_2 E_{22}^2 + a_4 E_{11} E_{22}) - 1 \right] \]

Tong and Fung (1976)

\[ -c \ln(1 - Q); \\
Q &= \frac{1}{2} c_1 E_{\theta\theta}^2 + \frac{1}{2} c_2 E_{zz}^2 + c_3 E_{\theta\theta} E_{zz} \]

Takamizawa and Hayashi (1987)

\[ c_{02}(I_4 - 1)^2 + c_{03}(I_4 - 1)^3 + e_{10}(I_1 - 3) + c_{11}(I_1 - 3)(I_4 - 1) + c_{20}(I_1 - 3)^2 \]

Humphrey et al. (1990a,b)

\[ \frac{c}{2} (\exp [c_1 (C_{11} - 1) + c_2 (C_{22} - 1) + c_3 (C_{33} - 1)] - 1) \]

Demiray and Vito (1991) for Media

\[ \frac{\mu}{2n} (\exp [\alpha (I_1 - 3)] - 1) \]

Demiray and Vito (1991) for Adventitia

\[ c_{0}(I_1 - 3) + \frac{1}{4} c (\exp(Q) - 1); \\
Q &= c_1 E_{rr}^2 + c_2 E_{\theta\theta} + c_3 E_{zz}^2 + c_4 E_{\theta\theta} E_{rr} + 2 c_5 E_{\theta\theta} E_{zz} + 2 c_6 E_{zz} E_{rr} \]

Holzapfel and Weizsäcker (1998)

\[ \frac{\mu}{2} (I_1 - 3) + \frac{k_1}{2k_2} \sum_{i=4,6} \left[ \exp(k_2 (I_i - 1)^2) - 1 \right] \]

Holzapfel et al. (2000)

\[ \frac{c}{2} [\exp(Q) - 1]; \\
Q &= A_1 E_{11}^2 + A_2 E_{22}^2 + 2 A_3 E_{11} E_{22} + A_4 E_{12}^2 + 2 A_5 E_{12} E_{11} + 2 A_6 E_{12} E_{22} \]

Sun and Sacks (2005)

\[ \frac{\mu}{2} (I_1 - 3) \mu I_m \left( (I_4 - 1) + J^I_m \ln \left( 1 - \frac{I_4 - 1}{J^I_m} \right) \right) \]

Horgan and Saccomandi (2005)

\[ \frac{\mu}{2} (I_1 - 3) + \frac{k_1}{2k_2} \left[ \exp \left\{ k_2 [\kappa I_4 + (1 - 3\kappa)I_1 - 1]^2 \right\} - 1 \right] \]

Gasser et al. (2006)

Table 1.1: List of isochoric strain energy density functions found in the literature for arterial tissue.
1.2.1.3 Biaxial Testing of Planar Soft Tissue Materials

Biaxial testing of planar materials has its modern roots in the work published by Rivlin and Saunders (1951) on the testing of nonlinear isotropic rubber materials at high strains. Biaxial tests offer an attractive method to determine the strain energy density function, \( \Psi \), of a hyperelastic material as explained below. In the general case of an isotropic material, \( \Psi \) is a function of three strain invariants, \( I_1 \), \( I_2 \) and \( I_3 \) (defined in Section 2.1.2.5). Typically, rubber is assumed to be incompressible implying that \( I_3 = 1 \) under any deformation. This reduces the number of invariants required to define \( \Psi \) to two. The principal Cauchy stress in terms of the principal stretches \( \lambda_i \), and the derivative of \( \Psi \) with respect to \( I_1 \) and \( I_2 \) is given in Equation (1.1).

\[
\sigma_i = 2 \left[ \frac{\lambda_i^2 \partial \Psi}{\partial I_1} - \frac{1}{\lambda_i^2 \partial I_2} \right] + p, \quad i = \{1, 2, 3\} \tag{1.1}
\]

where \( p \) is an indeterminate Lagrange multiplier which enforces incompressibility. A planar specimen under biaxial stretch is in a state of plane stress, hence \( \sigma_3 = 0 \). Hence the two planar principal Cauchy stresses may be defined as follows,

\[
\sigma_1 = 2 \left( \frac{\lambda_1^2}{\lambda_1^2 \lambda_2^2} \right) \left( \frac{\partial \Psi}{\partial I_1} \lambda_1^2 \frac{\partial \Psi}{\partial I_2} \right) + \lambda_1^2 \frac{\partial \Psi}{\partial I_2} \tag{1.2}
\]

\[
\sigma_2 = 2 \left( \frac{\lambda_2^2}{\lambda_1^2 \lambda_2^2} \right) \left( \frac{\partial \Psi}{\partial I_1} \lambda_2^2 \frac{\partial \Psi}{\partial I_2} \right).
\]

Assuming a homogeneous deformation, in a biaxial test the in-plane principal stretch and the Cauchy stress are determinable. The only unknowns are the derivatives of \( \Psi \) with respect to the strain invariants; these derivatives may be written as functions
Figure 1.2: Plots showing contours of A) constant $I_1$, and B) constant $I_2$ in biaxial principal stretch space $\lambda_1 - \lambda_2$ (assuming $\lambda_3 = 1/(\lambda_1 \lambda_2)$).

of the principal stretch and the principal Cauchy stresses.

$$\frac{\partial \Psi}{\partial I_1} = \frac{\lambda_1^2 \sigma_1}{\lambda_1^2 - 1/\lambda_1^2 \lambda_2^2} - \frac{\lambda_2^2 \sigma_2}{\lambda_2^2 - 1/\lambda_1^2 \lambda_2^2}$$

$$\frac{\partial \Psi}{\partial I_2} = \frac{\sigma_1}{\lambda_1^2 - 1/\lambda_1^2 \lambda_2^2} - \frac{\sigma_2}{\lambda_2^2 - 1/\lambda_1^2 \lambda_2^2}$$

Using Equation (1.3) the derivatives of $\Psi$ may be determined from experimentally measured data. Bearing in mind that the objective is to determine the functional form and model parameters of $\Psi$ for a given material, biaxial tests can be performed for constant values of $I_1$ and $I_2$, and plotted against the corresponding strain energy derivatives. Figure 1.2 demonstrates how the principal stretches must be varied in a biaxial test to maintain a constant value of $I_1$ or $I_2$. Four plots may be constructed from these data ($\partial \Psi_i/\partial I_j$, $i, j = 1, 2$ versus $I_1$ and $I_2$) and an appropriate functional form for $\Psi$ and the corresponding material parameters may be determined.

This is the framework as outlined in the paper by Rivlin and Saunders (1951).
Biaxial tests have been used extensively in biomechanics, starting with the pioneering work of Lanir and Fung (1974a,b) whose experimental setup is shown in Figure 1.3. The Rivlin framework outlined above was used by Humphrey et al. (1990a,b) to determine a strain energy function for passive myocardium using a transversely isotropic constitutive model which was a function of the isotropic invariant $I_1$, and an anisotropic invariant $I_4$ which is the square of the stretch of a reinforcing fibre. Analogous to Equation (1.3), the derivative of $\Psi$ with respect to the invariants is determined as a function of experimentally measured parameters. Biaxial tests at constant rates of $I_1$ and $I_4$ were performed and plots of the strain energy function derivatives versus the invariants constructed. The plots revealed that $\partial \Psi / \partial I_1$ increased linearly with increasing $I_1$, but decreased with increasing $I_4$. Next, $\partial \Psi / \partial I_4$ increased non-linearly with increasing $I_4$, and decreased linearly with $I_1$. Given these experimental observations, the following strain energy function was established;

$$\Psi = c_{02}(I_4 - 1)^2 + c_{03}(I_4 - 1)^3 + c_{10}(I_1 - 3) + c_{11}(I_1 - 3)(I_4 - 1) + c_{20}(I_1 - 3)^2 \tag{1.4}$$

for which the constants $c_{ij}$ were fit from the experimental data.

Lanir and Fung (1974a,b) investigated the mechanical properties of rabbit skin
using biaxial tests. Square specimens were mounted trampoline-like with as many as 68 attachment sites equally distributed along the four edges. Opposite actuators were mechanically connected such that they displaced at equal but opposite rates. Thus specimens could be stretched at different rates in different directions. Two video dimensional analyzers (VDAs) were used to measure the displacement between two points, both in the $x$ and $y$ directions. The importance of measuring strain in a central homogeneous region was acknowledged in this paper, as it allows for dissipation of any irregularities at the edges. In their review paper on biaxial testing, Sacks and Sun (2003) commented on the use of VDAs in this study:

“To avoid the effects of local stress concentrations of the suture attachments, bidirectional tissue strain was measured in a central region by monitoring the distance between pairs of lines separated by approximately 5 mm along each axis video dimensional analyzers (VDAs).”

At this early stage in the history of biaxial testing of biomaterials it was acknowledged that there is stress and strain inhomogeneity in biaxial specimens. The solution proposed was to measure strain in a region of assumed homogeneity. However, no comment was made on how this inhomogeneity effects the calculation of stress in a biaxial specimen.

The experiments of Lanir and Fung (1974a,b) demonstrated some important key characteristics of soft tissues: $i$) that skin displays a non-linear anisotropic stress-strain relationship, and $ii$) that differences were observed between loading and unloading curves. In this particular case the skin did not exhibit a dependence on strain rate. This experimental data was then used to determine a constitutive model for skin, with the material parameters being determined by matching specific points on the stress-strain curves (Tong and Fung, 1976). The authors take care to use appropriate stress and strain measures in the correct configuration (be it deformed/undeformed) when analysing the experimental data.
The work of Vito and co-workers is credited with making the next substantial improvement in biaxial tests of biomaterials. To improve the measurement of strain in the specimen, multi-particle tracking was employed. This method tracked a 2D element on the specimen and allowed the calculation of the in-plane deformation gradient, including the shear components. Use of real-time computer controls for the machine actuators enabled strain controlled experiments (Vito, 1980).

Importantly, a technique was developed by Choi and Vito (1990) where the principal material axis of a biaxial specimen could be determined non-destructively. A circular specimen of tissue is prepared, and marks on its edge are made at 15° intervals. The specimen is clamped at two opposing marks and loaded up to a defined value; when this is reached two marks are made aligned to the stretch axis. The specimen is rotated and the procedure repeated. On completion, an ellipse is outlined on the specimen, the major and minor axis of which are the principal material directions. This represented an improvement on previous work which is based on gross anatomy Choi and Vito (1990); Demiray and Vito (1991).

Interestingly Choi and Vito (Choi and Vito, 1990) encountered problems regarding the reproducibility of experiments when strain-control was used, as opposed to force-control. Returning to the review of Sacks and Sun (2003), on this topic they comment that “The reason underlying this disagreement is at present unknown and suggests a need for experimental and theoretical investigations of constitutive theories that can better handle mixed boundary conditions.”

To gain further insight into the fibrous structure of soft anisotropic tissues, a small-angle light scattering (SALS) method has been used effectively (Billiar and Sacks, 1997; Waldman et al., 2002; Sacks et al., 1997). SALS allows for the point-wise measurement of fibre angles in a specimen. Using this technique, a preferred fibre direction can be calculated and more homogeneous specimens tested. The application of this method to biaxial tests on bovine pericardium (Sacks and Chuong,
1998) led to a consistent mechanical response and low variability in the material parameters. The use of SALS to control for specimen structure represents an improvement on previous methods which were based on visual inspection.

One assumption which is commonly made for biaxial tests is that in-plane shear is negligible. This assumption is acceptable provided that the material axes of the specimen in question are aligned with the axes of stretch. However, shear deformation of tissues is a biomechanically relevant mode of loading and warrants investigation. The controlled imposition of an in-plane shear deformation is practically challenging. Some investigators have used individual actuators connected to single points along the boundary of the specimen to impose shear deformation (Flynn et al., 1998; Khalsa et al., 1996). Others have adapted standard biaxial machines, using rotating carriages to impose a multiaxial stress state on a specimen, from which the shear stress-strain behaviour is parsed (Sacks and Chuong, 1998; Sacks, 1999). The latter setup was used to investigate the mechanics of bio-prosthetic heart valve materials subjected to large in-plane shear (Sun et al., 2003).

Finally, a study by Nielsen et al. (1991) was one of the first to critically review the experimental setups used for biaxial tests, and to implement some improvements in the experimental equipment used. Importantly, a finite element study of a biaxial test (simulating an isotropic material) was used to assess the uniformity of the stress and strain field. They concluded that stress and strain were uniform within a small region in the centre of a specimen. Improvements in the measurement of the strain field in a biaxial specimen have been made subsequently (Malcolm et al., 2002). A computational study assessing the uniformity of the stress and St. Venant effects in clamped and sutured, square and cruciform specimens was performed (Sun et al., 2005). It was shown that significant stress inhomogeneity exists in biaxial specimens and noted that boundary effects are strongest in square clamped specimens. It was recommended that sutured square specimens be used, whilst stating that this setup
too resulted in a high level of stress inhomogeneity. Sutured specimens have been shown to be susceptible to unpredictable stress concentrations, due to the irregular nature of the spacing of attachments (Eilaghi et al., 2009). Recognising this, inverse FE methods (Krishnamurthy et al., 2008), and correction factors (Jacobs et al., 2013) have been proposed to circumvent this problem.

1.2.1.4 Compressibility of Arterial Tissue

Arterial tissue has been assumed to be incompressible in contemporary biomechanics studies since the initial work of Lanir and Fung (1974a). From a mechanistic perspective, this assumption is convenient as it simplifies the interpretation of experimental data and the solution of theoretical problems. As many of the first hyperelastic constitutive laws used in biomechanics are based on earlier work on rubber materials, which are commonly treated as incompressible, this assumption was a convenient choice.

The assumption of arterial incompressibility is not based solely on convenience; some early experimental studies suggested that the assumption is valid. The first study on arterial compressibility by Lawton (1954) determined that stretching of an artery wall was an isovolumetric process. The first study to implement an imaging technique (Dobrin and Rovick, 1967) used X-ray images of the cross-section of canine carotid arteries to determine a change in thickness in the vessel wall in an inflated and uninflated state. The study determined that the volume of the wall did not change upon inflation. Tickner and Sacks (1967) also used an X-ray technique to determine the cross-sectional area of various human and animal arteries. A number of different pre-stretches and internal pressures were examined. Interestingly, this study found decreases in the volume of the artery wall of up to 35%. This was the first study to suggest that arterial tissue is compressible.

The study by Carew et al. (1968) was the first study to focus solely on the
compressibility of arterial tissue, and arguably has been the most influential study on arterial compressibility with over 420 citations at the time of writing. Figure 1.4 shows a schematic of the experimental setup. The study was based on the change in water level of a tank in which a submerged straight artery segment is inflated and deflated under physiological loading conditions. The compressibility of the tissue was determined by calculating the ratio of the bulk modulus to the shear modulus. To calculate the bulk modulus, the volumetric strain was determined from the change in volume of the artery segment, and the hydrostatic stress from the axial force and internal pressure together with the Laplace equation. The shear modulus was taken from the literature. Though experimental data in this paper suggests compressibility, the authors concluded that at small strains the assumption of incompressibility is valid.

The issue of arterial compressibility was investigated by Y.C. Fung (Chuong and Fung, 1984) several years later. A different approach to the above papers was taken in this study. Square or rectangular flat specimens of rabbit thoracic aorta were placed between two glass slides and subjected to a uniaxial compression in the material radial direction. A camera was positioned such that it could image the underside of the specimen (i.e. took images of the $\theta - z$ plane). These images were used to measure the tissue strain and the fluid exudation from the specimen, which
occurred as a result of the applied compression. The paper concludes that very little fluid is lost from the vessel wall during compression, and that these data support the incompressibility hypothesis. However, no attempt was made to measure the precise geometric deformation of the specimen before and after loading. The results of this study too are often cited in the literature as verification that the incompressibility hypothesis is correct (currently > 150 citations).

A more recent study used ultrasound (Girerd et al., 1992) to measure incompressibility of human mammary and radial arteries, in vitro, at physiological pressures. The ultrasound measured the cross-sectional area of the arteries at systole and diastole and found that there was no change in area. It should be noted however that no change in area does not necessarily mean that there is no change in volume and vice versa.

Some studies have attempted to measure changes in vessel volume in vivo using video-dimension analysis of transilluminated vessels (Faury et al., 1999), and Chesler et al. (2004) using transillumination with an inverted microscope. These studies found 15–20% compressibility in arteries.

A novel method proposed by Volokh (2006) involved using the change in geometry observed in artery ring cutting experiments, due to the release of residual stress, to determine compressibility of arterial tissue. However geometry changes are small and may be difficult to measure in practice.

In addition to writing a review on the state-of-the-art on investigations of arterial compressibility, Di Puccio et al. (2012) proposed a modified apparatus based on the work of Carew et al. (1968). The apparatus consisted of a PMMA outer tube filled with saline solution into which an artery is placed. The artery is sealed from the outer tube and can be inflated independently with saline. The volume change of the vessel was measured by measuring the volume of saline pumped into the vessel, versus the volume of water displaced from the outer tube - which was measured
using a capillary tube. A drop of mercury was added to the tubing which fed saline into the artery, serving as a marker to indicate volume change. A dye was also used to check for any leakage from the artery to the outer tube. Di Puccio et al. (2012) examined only two specimens and found volume changes of up to 6% at physiological pressure, and 20% at supra-physiological pressures.

Yosibash et al. (2014) proceeded to construct the experimental apparatus outlined by Di Puccio et al. (2012). Porcine saphenous \( (n = 5) \), femoral \( (n = 6) \), and carotid \( (n = 1) \) arteries were tested. Pressure–volume change plots show a volume change of between 1-3% at physiological pressures, and up to 10% at supra-physiological pressure. An empirical equation was fit to the data of the form,

\[
\frac{\Delta V}{V_0} = P^{a_A} \exp(b_A V_0) \exp(c_A) - P^{a_R} \exp(b_R V_0) \exp(c_R) \tag{1.5}
\]

where \( \frac{\Delta V}{V_0} \) is the volume change, \( P \) is the intraluminal pressure, and \( a_A, b_A, \) and \( c_A \) are parameters determined from the experimental data for arterial tissue and \( a_R, b_R, \) and \( c_R \) are parameters determined from the experimental data for rubber.

Comment on radius measurement to determine volume change in lumen pressure experiments

In practical terms, it is quite difficult to determine the volume change in tube based on its radius. The equation for the volume change in a tube with fixed ends is,

\[
\frac{\Delta V}{V_0} = \frac{r_o^2 - r_i^2}{R_o^2 - R_i^2} - 1 \tag{1.6}
\]

where \( R_o \) and \( R_i \) are the undeformed outer and inner radius, and \( r_o \) and \( r_i \) are the
Figure 1.5: Plot of the percentage change in outer radius $r_c$ of a compressible artery inflated to 1.2 times its inner radius for a given percentage volume change, $\Delta V/V_0$. The outer radius is normalised by its incompressible counterpart $r_{ic}$.

deformed outer and inner radius. The volume change has approximately a square relationship with the radius, meaning that a small change in radius will have a large influence on the volume change calculated.

A simple example is now used to demonstrate this. For the undeformed geometry $R_o = 12$ and $R_i = 9$ are used. For the deformed configuration the inner radius is increased to $r_i = 1.2 R_i$. Then the deformed outer radius is calculated for a prescribed volume change. Results are plotted in Figure 1.5 where $r_c$ is the outer radius of a compressible artery, $r_{ic}$ is outer radius of an incompressible artery. From this plot we can see that a 1% change in measurement of radius leads to a 5-6% change in calculated volume. It’s clear that measuring volume change from measurement of radii/cross-sectional areas is a technique prone to errors.
Figure 1.6: MicroCT scan images of human trabecular bone from the proximal femur and the vertebra. The images are of the same resolution and macro dimensions. It is immediately clear that the structure of TB is heterogeneous and that there is a substantial difference in structure between anatomical sites. The basic plate-like and rod-like structural components of bone are visible particularly in image (Keaveny et al., 2001).

1.2.2 Biomechanics of Hard Tissue

In addition to investigating the anisotropic behaviour of soft tissue at large strains, this thesis also investigates the anisotropic behaviour of hard tissue at large strains. Specifically, trabecular bone is considered. Here a background of bone biomechanics and inelastic behaviour is presented. In the specific study of trabecular bone (TB), the primary areas of interest are risk identification in age related bone fracture and bone-implant mechanics (Keaveny et al., 2001).

In order to understand the mechanics at the bone-implant interface (micro level), one must determine the stress and deformation in the surrounding TB tissue during press-fit implantation of orthopaedic devices. There are no viable experimental methods for measuring the stress state during implantation and the problem is far too complex for analytical solutions. Therefore representative, accurate constitutive models and their finite element (FE) implementation offer a valuable method for the analysis and design of orthopaedic implants.
1.2.2.1 Structure of Trabecular Bone

From an engineering perspective, TB, like many other biological tissues, is a remarkably complex material. TB is the porous, spongy bone which is found at the ends of all long bones and in some irregular bones such as the pelvis and vertebrae (Cowin, 2001). Using the analogy to cellular solid engineering materials, TB is an open-celled foam where the pore sizes are on the order of 1 mm and the connecting struts are on the order of 100 µm. Figure 1.6 shows a microCT image of trabecular bone from two different anatomical locations and shows the porous nature of bone. Typically TB struts are structurally aligned with predominant loading directions, providing enhanced strength and stiffness in critical directions (Cowin, 2001; Keaveny et al., 2001). This results in material anisotropy at a continuum level (Katz and Meunier, 1987).

The TB tissue from which the struts are constructed is in itself a complex engineering material. Figure 1.7 shows that at the nano-scale, TB is formed from collagen fibrils which have been mineralised by hydroxyapatite crystals (a naturally occurring form of calcium carbonate). These fibrils band together uni-directionally to form lamellar bone sheets and it is from cross-ply combinations of lamellar bone sheets that trabecular bone sheets are formed (Vaughan et al., 2012). Bone volume fraction and trabecular alignment varies spatially throughout a bone, resulting in highly heterogeneous material behaviour (Goldstein, 1987).

1.2.2.2 Experimental determination of mechanical properties

It is widely recognised that material properties are spatially heterogeneous within a single bone (Goldstein, 1987; Keaveny et al., 2001). To achieve a large enough sample size, specimens from multiple animals must be obtained, hence introducing the problem of cross-subject variability (Cowin, 2001). The machining of specimens into a required shape interrupts the trabecular network and allows damage to be
induced more easily at the faces where the testing platens are in contact with the specimen (Røhl et al., 1991). It is clear that mechanical testing of trabecular bone is non-trivial.

Early work investigating the modulus and compressive strength of bone was performed by Linde and co-workers (Røhl et al., 1991; Linde et al., 1991). Problems in calculating mechanical properties were identified due to the miscalculation of strain during tests (Odgaard and Linde, 1991). Odgaard and Linde (1991) hypothesised that the reason for this was that the external trabecular struts underwent damage due to their being exposed, thus causing an apparent increase in strain and therefore decreasing modulus. The macro-scale tension/compression asymmetry in bone was also identified (Røhl et al., 1991), the compressive strength was $2.22 \pm 1.42$ MPa and the tensile strength $2.54 \pm 1.18$ MPa.

In the early 1990s Keaveny and co-workers investigated the elasticity of trabecular bone. Cylindrical specimens with a height/diameter ratio (aspect ratio) of approximately 2:1 were used, which minimises the amount of exposed trabecular struts on a given specimen (Keaveny et al., 1994b, 2001). An additional improvement was the use of reduced cross-sectional area (dog-bone) specimens with an extensometer attached to the gauge length. The benefit of this technique is that any unrepresentative deformations at the attachment site are negated, and that failure should occur
Figure 1.8: Correlations taken from Keaveny et al. (1994b). These figures show a strong relationship between strength and modulus and a reasonable correlation between strength and apparent density.

at the reduced cross-section (Keaveny et al., 1994b). A further improvement was to use contact radiographs to select specimens which had a trabecular architecture that was aligned with the long axis of the specimen, thus ensuring consistent on-axis loading of the specimens (Keaveny et al., 1994a).

The result of these improvements in experimental protocol was to show that some of the previously reported phenomena were experimental artefacts. The non-linear toe region at the start of the stress-strain curve is not observed. The modulus of TB is equal in tension and compression (Keaveny et al., 1994a). One finding which contradicted the findings of Røhl et al. (1991), was that the apparent yield strength was greater in compression than in tension (Keaveny et al., 1994b). Figure 1.8 shows that a correlation between bone density and yield strength was found and a strong correlation between modulus and yield strength was revealed.

Ford and Keaveny (1996) hypothesized that the failure strains in TB are homogeneous and isotropic. Cylindrical, reduced cross-section specimens of bovine TB were tested in torsion with two sample groups. One sample group was tested parallel to its on-axis direction, while the other was tested perpendicular to its on-axis direction. Figure 1.9 plots a representative shear stress–shear strain curve for bovine TB. The failure (yield and ultimate) stresses were highly scattered, though failure stresses in the on-axis orientation were found on average to be 1.61 times greater
than in off-axis specimens. Failure strains were more closely distributed than the failure stresses within both the longitudinal and the transverse sample groups.

A table of mechanical properties of trabecular bone, found in literature, is given in Figure 1.10.

1.2.2.3 Micromechanical finite element models

In the mid-nineties technological advances occurred in the fields of computational modelling and medical imaging. This made the micromechanical FE analysis of TB feasible. Work by van Rietbergen et al. (1995) a 3D voxel FE mesh was created by serially sectioning a trabecular bone specimen and taking high quality digital photographs of each section. A voxel mesh provides an approximation of the 3D geometry using regular cuboidal shaped hexahedral elements. An artefact of voxel based modelling is that exposed curved surfaces of the bone are not replicated. Instead of a smooth surface, a best-fit zig-zag series of discrete steps approximates the surface geometry, as shown in Figure 1.11. Typically the number of elements in a mesh was on the order of $10^5$ (Keaveny et al., 2001). Material properties are applied to the tissue, and boundary conditions to the mesh to predict macro-scale mechanical behaviour (Niebur et al., 1999). An initial study aimed to find the elastic modulus of the bone tissue which would result in the same apparent level modulus
<table>
<thead>
<tr>
<th>Author</th>
<th>Year</th>
<th>Species</th>
<th>Site</th>
<th>Young’s Modulus (MPa)</th>
<th>Yield Strength (MPa)</th>
<th>Ultimate Strength (MPa)</th>
<th>Yield Strain (%)</th>
<th>Ultimate Strain (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Morgan</td>
<td>2001</td>
<td>Human</td>
<td>Vertebra</td>
<td>344 ± 148 (C) 349 ± 133 (T)</td>
<td>2.02 ±0.92 (C) 1.72 ±0.64 (T)</td>
<td>-</td>
<td>0.77 ±0.06 (C) 0.70 ±0.05 (T)</td>
<td>-</td>
</tr>
<tr>
<td>Morgan</td>
<td>2001</td>
<td>Human</td>
<td>Proximal tibia</td>
<td>1091 ± 634 (C) 1068 ± 840 (T)</td>
<td>5.83 ± 3.42 (C) 4.50 ± 3.14 (T)</td>
<td>-</td>
<td>0.73 ±0.06 (C) 0.65 ±0.05 (T)</td>
<td>-</td>
</tr>
<tr>
<td>Morgan</td>
<td>2001</td>
<td>Human</td>
<td>Greater trochanter</td>
<td>622 ± 302 (C) 597 ± 330 (T)</td>
<td>3.21 ± 1.83 (C) 2.44 ± 1.26 (T)</td>
<td>-</td>
<td>0.70 ±0.05 (C) 0.61 ±0.05 (T)</td>
<td>-</td>
</tr>
<tr>
<td>Morgan</td>
<td>2001</td>
<td>Human</td>
<td>Femoral neck</td>
<td>3230 ± 936 (C) 2700 ± 772 (T)</td>
<td>17.45 ± 6.15 (C) 10.93 ± 3.08 (T)</td>
<td>-</td>
<td>0.85 ±0.10 (C) 0.61 ±0.03 (T)</td>
<td>-</td>
</tr>
<tr>
<td>Ford</td>
<td>1996</td>
<td>Bovine</td>
<td>Proximal tibia</td>
<td>2470 ± 798 (L) 719 ± 241 (Tr)</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Ashman</td>
<td>1987</td>
<td>Bovine</td>
<td>Femur</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Garnier</td>
<td>1999</td>
<td>Human</td>
<td>Proximal femur</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Garrison</td>
<td>2011</td>
<td>Bovine</td>
<td>Proximal tibia</td>
<td>2102 ± 711</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Keaveny</td>
<td>1993</td>
<td>Bovine</td>
<td>Proximal tibia</td>
<td>2380 ± 777 (C) 2630 ± 727 (T)</td>
<td>21.3 ± 8.05 (C) 15.6 ± 4.19 (T)</td>
<td>23.6 ± 8.28 (C) 16.9 ± 4.24 (T)</td>
<td>1.09 ±0.12 (C) 0.78 ±0.04 (T)</td>
<td>1.86 ±0.49 (C) 1.37 ±0.33 (T)</td>
</tr>
<tr>
<td>Rincon-Kohli</td>
<td>2009</td>
<td>Human</td>
<td>Multiple sites</td>
<td>598 ± 401 (C) 755 ± 454 (T)</td>
<td>8.97 ± 7.57 (C) 3.37 ± 1.93 (T)</td>
<td>10.16 ± 8.92 (C) 4.02 ± 2.34 (T)</td>
<td>1.52 ±0.36 (C) 0.67 ±0.10 (T)</td>
<td>2.31 ±0.77 (C) 1.41 ±0.01 (T)</td>
</tr>
</tbody>
</table>
Figure 1.11:  A) Voxel mesh of a section of trabecular bone, note the regular size and uniform orientation of the elements [1].  B) A schematic showing how tissue level tensile strains can arise in trabecular bone under a compressive apparent strain, due to its irregular geometry (van Rietbergen et al., 1995).

as observed in experimental studies (van Rietbergen et al., 1995). A linear elastic constitutive model was assigned to the tissue, with an assumed Poissons ratio of 0.3. For an apparent level modulus range of between 88-400 MPa, the tissue level modulus ranges between 2.2 - 10.1 GPa (van Rietbergen et al., 1995).

An advantage of micromechanical modelling is the quantification of the local stress and strain fields in the TB architecture. Simulations reveal equal quantities of elements in tensile and compressive strain, with a slight bias towards compressive strain in the direction of uniaxial compression. This indicates that bending of trabeculae occurs at the microstructural level, despite the uniaxial compression at the apparent level (Niebur et al., 2000; van Rietbergen et al., 1995) (see Figure 1.11B). An analysis of the von Mises stress distribution in the model reveals that the majority of trabeculae carry load (van Rietbergen et al., 1995).

The study by Niebur et al. (2000) took this technique one step further by carrying out specimen specific combined experimental and computational studies. A tissue modulus for each individual specimen was found by calibrating a linear FE analysis. Motivated by the hypothesis that TB tissue may behave like cortical bone; a strength asymmetric, bilinear elastic constitutive model was assigned to the trabecular tissue and a non-linear analysis was completed. Predictions of the specimen
specific apparent level yield stress and strain were remarkably close to the experimental values.

Recent microstructural FE models have used site specific material properties for the trabecular tissue material determined using nano-indentation (Harrison et al., 2008). Models for bone damage have also been introduced. Harrison et al. (2013) presented a damage model for vertebral TB specimens in uniaxial compression, using a principal strain based criterion and simulating fracture through element deletion and cohesive forces in the trabecular microstructure.

1.2.2.4 Yield criteria for trabecular bone

A number of yield criteria for TB have been proposed in the literature. Early criteria were based on experimental data (Fenech and Keaveny, 1999; Keaveny et al., 1999; Rincón-Kohli and Zysset, 2009), and when the computational methods described in Section 1.2.2.3 became more accepted as a substitute for direct experiments, several more yield criteria emerged for multiaxial loading (Bayraktar et al., 2004; Cowin and He, 2005; Garcia et al., 2009; Gupta et al., 2007).

An initial attempt to find a yield criterion for TB used the Tsai-Wu yield criterion, which was developed for cellular solids (Fenech and Keaveny, 1999). The model was calibrated using experimental data from compression, torsion and triaxial tests on specimens of TB. A large spread in mechanical properties due to factors such as structural heterogeneity and bone density was observed. The calibration of the Tsai-Wu model is challenging because of the large number of coefficients which are required, and the dominance of one of the terms in the yield function which greatly influences the orientation of the yield surface.

Normalization of the yield stress by the Young’s modulus, effectively giving the yield strain, was shown to offset the heterogeneous effects due to bone density (Fenech and Keaveny, 1999). Figure 1.12 shows the yield points in the shear
Figure 1.12: Plot of yield stresses which have been normalized by modulus. These are the result of biaxial mechanical tests on cylindrical specimens of TB. A clear failure envelope began to emerge from this analysis and the cellular solid yield criterion was developed (Fenech and Keaveny, 1999). The plot also shows the Tsai-Wu yield criterion and demonstrates its inability to capture this multiaxial data.

stress-unaxial stress plane, determined from multiaxial stress tests on TB. A clear failure envelope emerges in this analysis and the Cellular Solid yield criterion was formulated to model this data (Fenech and Keaveny, 1999). The failure envelope is more accurately captured by the Cellular Solid yield criterion than by the Tsai-Wu criterion.

Follow-up work by Kopperdahl and Keaveny (1998) focused on the yield strains of both human vertebrae (low density) and bovine tibia (high density) TB. Tensile specimens had a consistent yield strain of approximately 0.78%, independent of anatomic site and density. The results of the compression testing were less conclusive. Low density specimens yielded at strains close to those observed in tension (0.84%), with a linear dependence of compressive yield strain on apparent density. The consistency of yield strains for higher density specimens could not be definitively determined.

This motivated the creation of a strain-based yield criterion for trabecular bone using finite element micromechanical models. In the study by Bayraktar et al. (2004), three specimens of TB were imaged using microCT. Voxel meshes were created from the scans and the tissue properties calibrated using the data from the
mechanical testing. For each specimen 266 different normal strain and 81 normal-shear strain loading paths were analysed, and a yield surface established as shown in 1.13A.

The yield strains were plotted in strain space and it was decided that a super-ellipsoid fitted the data best. The authors developed a 4 parameter modified super-ellipsoid yield criterion which described the yield data well, while minimising the number of parameters necessary to calibrate the model (Figure 1.13B). The arithmetic error of the fit of yield surface to the principal strain yield data was $-0.04 \pm 5.10\%$, and an excellent fit to the axial-shear data was also achieved with an error of $2.5 \pm 6.5\%$.

Fabric tensors have been used to model density and morphology dependent anisotropic elasticity Zysset (2003). Likewise they have been utilised to construct yield criteria which account for bone architecture and apparent density (Garcia et al., 2009; Wolfram et al., 2012; Zysset and Rincón, 2006). Zysset and Rincón (2006) formulated a complex yield surface, which they named the piecewise Hill model. It is based on fourth order tensors which intrinsically incorporate the axial and shear strengths as well as fabric eigenvectors as parameters. As seen in Figure 1.14A, the yield surface is discretised into two portions, separated by a hyperplane which demarcates the tensile and compressive zones.
The model was calibrated using morphological and mechanical experimental data. The unique aspect of this yield criterion is that its shape is largely determined by the morphology. When the quality of the fit to the experimental data was analysed it was found that for certain multiaxial modes of loading, yield prediction was poor.

Wolfram et al. (2012) developed a fabric based Tsai-Wu yield criterion in both stress and strain space. The yield surfaces were formulated using a complex mix of second and fourth order fabric tensors where material constants are power law functions of apparent density and fabric orientation. A damage coefficient was adopted into the strain space yield criterion. This was used as a correction factor to allow the stress yield criterion to be transformed into the strain based criterion via the compliance tensor. The authors state there is good correlation between predicted and measured values of yield, with a standard error and concordance correlation coefficient of 5.47% and 0.93 respectively in strain space and 13.58% and 0.96 in stress space. The stress space yield surface is shown in Figure 1.14B with experimental data superimposed.

Figure 1.14: A) The piecewise Hill model from Rincón-Kohli and Zysset (2009) and B) the fabric based Tsai-Wu criteria of Wolfram et al. (2012) in normalized principal stress space.
1.2.2.5 Plasticity models for trabecular bone

The predominant focus of macro-scale orthopaedic biomechanics over the past two decades has been on accurately characterising the multiaxial elastic behaviour of TB. In contrast, the plasticity of TB has been relatively neglected though there are plasticity models which have been specifically formulated for TB (Garcia et al., 2009; Gupta et al., 2007; Papadopoulos and Lu, 2001).

Gupta et al. (2007) developed a strain space plasticity model based on the modified super-ellipsoid of Bayraktar et al. (2004). Though the plasticity formulation was developed in strain space, many of the same features exist as for plasticity models in stress space. The evolution of the yield is described by several equations such as the yield function, flow rule and consistency condition, except that these functions are phrased in terms of strain. A Newton–Raphson scheme was devised to solve these equations and a consistent tangent matrix was formulated. This formulation uses simple uniform hardening and was never compared to multiaxial inelastic data.

A plasticity model was developed by Garcia et al. (2010) for modelling the cyclic behaviour of cortical bone. Figure 1.15 shows a one-dimensional rheological model for the plasticity formulation. It consists of a linear spring to represent the elastic regime, a damageable spring and a plastic pad represent the inelastic behaviour of the material. A damage variable exists for the second spring which accounts for microcracks in the bone. It acts by decreasing the stiffness of the spring which is in parallel with the plastic pad, thereby representing weakening of the material. A generalization to three dimensions is made in a follow-up study (Garcia et al., 2009). However, this model considers only isotropic hardening and does not compare its predictions of inelastic material behaviour to any experimental data.

An over-nonlocal plasticity model based on the constitutive model by Garcia et al. (2009) was developed by Hosseini et al. (2015). This model eliminates the effects of mesh size on the prediction of internal damage and plasticity variables.
and increases computational efficiency. However it does not specifically address the modelling of post-yield behaviour.

The study by Kelly and McGarry (2012) was the first to specifically address the macro-scale post-yield behaviour of TB using a pressure-dependent Crushable-Foam yield function. It was demonstrated that von Mises, Drucker-Prager, and Mohr-Coulomb models fail to predict the multiaxial inelastic behaviour of TB. Instead, Kelly and McGarry (2012) recommend that a Crushable-Foam type model (Deshpande and Fleck, 2000) with isotropic hardening should be used to predict inelastic behaviour, and demonstrate its efficacy in modelling both uniaxial and confined compression inelastic behaviour.
Bibliography


ADINA, R. Inc. adina theory and modeling guide. Reports ARD 97–7; 97, 8, 2005.


Chapter 1


Chapter 2

Theory

The engineering don is apt to pretend that to get anywhere worthwhile without the higher mathematics is not only impossible but that it would be vaguely immoral if you could.

J.E. Gordon - *Structures: or why things don’t fall down*

2.1 Continuum Mechanics

Continuum mechanics provides the theoretical foundation upon which much of the current research is based. A thorough foundation in this topic is required for the development of non-linear constitutive laws, especially those involving finite deformations. As its name suggests, continuum mechanics treats a body as a continuous entity which can be described by smooth functions of spatial variables. The general approach in continuum mechanics is to formulate mathematical models which describe the macroscopic mechanical behaviour of fluid and solids. This section outlines the essential elements of continuum mechanics required for the interpretation of the subsequent chapters.
2.1.1 Deformation and Motion

The classic representation of deformation and motion is outlined in Figure 2.1. Here, the undeformed/Lagrangian configuration of a body whose domain is $\Omega_0$, at time $t = 0$ is considered. To describe deformation and motion, equations must be stated with respect to a reference configuration. It is often logical and mathematically convenient to use this undeformed configuration as this reference configuration. As the body undergoes deformation, displacement, or a combination of both, it is in the deformed/Eulerian configuration, whose domain is $\Omega$.

The position of a material point $P$ in the reference configuration, with respect to the origin, is denoted by the vector $X$. The coordinates of $P$ and hence $X$ in the
reference configuration do not change as a function of time. A vector such as $X$ can be described for all points within the domain $\Omega_0$. Such vectors are known material coordinates or Lagrangian coordinates. Likewise for the current configuration, a vector $x$ may be defined which describes the location of material point $P$. The coordinates of $x$ give the spatial position, and are known as the spatial or Eulerian coordinates. The motion or transformation of the body from the undeformed to the deformed configuration is described by the equation,

$$x = \chi(X, t),$$

(2.1)

where $\chi$ is a vector mapping function from the initial to the current configuration.

As this thesis is primarily concerned with solid mechanics, the material or Lagrangian description of displacement is used where the independent variables are the material coordinates $X$ and the time $t$. It is clear from Figure 2.1 that displacement, $u$, of a material point $P$ from the initial to the deformed configuration is described by the equation, $u = x - X$. Combining this with Equation 2.1 results in an expression for $u$ in terms of $X$ and $t$,

$$u = \chi(X, t) - X$$

(2.2)

The rigid body kinematics of a body are not of specific interest here, rather the quantification deformation and strain in a body is. An essential building block to calculating this is second order tensor known as the deformation gradient, it is defined as,

$$F = \frac{\partial \chi}{\partial X} = \frac{\partial x}{\partial X} = (\nabla \chi)^T,$$

(2.3)
where $\nabla_0$ is the left gradient operator with respect to the material coordinates. Consider an infinitesimal vector $dX$ in the undeformed configuration (see figure 2.1). Equation 2.3 is defined such that,

$$dx = F \, dX.$$  \hfill (2.4)

The determinant of $F$ is known as the Jacobian of the deformation gradient, and is often used to relate the undeformed and deformed configurations. In addition it also denotes the ratio of the volume change, from the undeformed to deformed configurations, in an infinitesimal volume element in a body,

$$J \equiv \det(F) = \frac{dV}{dV_0},$$  \hfill (2.5)

where $dV_0$ is the infinitesimal element volume at the undeformed configuration and $dV$ at the deformed configuration.

The validity of the above equations is subject to three criteria. Firstly, the mapping function $\chi(X, t)$ must be continuously differentiable or in special circumstances piecewise differentiable. Secondly, the mapping function must map a unique point on the reference configuration to a unique point on the deformed configuration. The reverse must also be possible. The final condition is that $J > 0$. This is obvious if one imagines that a body cannot have a volume of zero or less. Theoretically, it ensures that the deformation gradient is invertible.

The derivative of the spatial velocity, $v = \partial u/\partial t$, with respect to the spatial coordinates is given as

$$L = \frac{\partial v}{\partial x},$$  \hfill (2.6)
The non-symmetric second order tensor $\mathbf{L}$ is known as the spatial velocity gradient. It can also be calculated using the deformation gradient $\mathbf{F}$:

$$
\mathbf{L} = \dot{\mathbf{F}} \mathbf{F}^{-1}
$$

where $\dot{\mathbf{F}}$ is the time derivative of the deformation gradient. The spatial velocity gradient is commonly additively decomposed into symmetric and skew-symmetric parts,

$$
\mathbf{D} = \frac{1}{2}(\mathbf{L} + \mathbf{L}^T) = \text{sym}(\mathbf{L})
$$

$$
\mathbf{W} = \frac{1}{2}(\mathbf{L} - \mathbf{L}^T) = \text{asym}(\mathbf{L})
$$

The symmetric part, $\mathbf{D}$, is the rate of deformation tensor, and the skew-symmetric/anti-symmetric part, $\mathbf{W}$, is the spin tensor.

### 2.1.2 Strain Measures

The deformation gradient $\mathbf{F}$ is the fundamental building block used to define motion/deformation in finite deformation problems. However, as engineers, we are more familiar with the concept of strain, which in its most elementary form is defined as the change in length of an element divided by its original length ($\varepsilon = \Delta l/l_0$) in the case of a one dimensional deformation. There are a variety of different strain/deformation measures which can be constructed from the deformation gradient.
In this section, second order deformation/strain tensors in lowercase bold are in the deformed/Eulerian configuration (e.g. $b$), while tensors in uppercase bold are the undeformed/Lagrangian configuration (e.g. $C$).

### 2.1.2.1 Stretch Ratio

First, imagine a unit vector $a_0$ in the undeformed configuration. This vector may be mapped to the deformed configuration by the deformation gradient. The resultant of this mapping is the stretch vector $\lambda a_0$ and is defined as,

$$\lambda a_0 = Fa_0,$$

(2.10)

where the length of the stretch vector, $\lambda$, is named the stretch ratio. The stretch ratio can be considered a unit of strain as it gives us an indication of the change in length of an element. However it has one inconvenient characteristic; that is that $\lambda = 1$ when it is unstretched i.e. when there is no deformation.

### 2.1.2.2 Deformation Tensors

If one computes the square of the stretch ratio $\lambda$, the following emerges,

$$\lambda^2 = \lambda a_0 \cdot \lambda a_0 = Fa_0 \cdot Fa_0$$

$$= a_0 \cdot F^T Fa_0 = a_0 \cdot Ca_0,$$

(2.11)

where

$$C = F^T F,$$

(2.12)
is the right Cauchy–Green deformation tensor, which is defined in Lagrangian/ material coordinates. It is a symmetric second order tensor. The right Cauchy–Green deformation tensor is often used in hyperelastic and hyper-elasto-plastic constitutive laws as a fundamental measure of deformation. The Eulerian/spatial counterpart to the right Cauchy–Green deformation tensor is the left Cauchy–Green deformation tensor \( b \). It is derived in a similar manner and is given as,

\[
 b = FF^T. \tag{2.13}
\]

The left Cauchy–Green tensor too is symmetric and positive definite. Though they measure the deformation in a body and are often used in constitutive models, the Cauchy–Green deformation tensors are not strain measures in the sense that they are non-zero in the initial configuration.

### 2.1.2.3 Strain Tensors

A commonly used strain measure is the Green–Lagrange strain \( E \) defined as,

\[
 E = \frac{1}{2}(C - I). \tag{2.14}
\]

The use of one half in the definition is to maintain consistency with small-strain theory, and indeed under small deformations the Green–Lagrange strain tensor results in the small-train tensor. As \( C \) and \( I \) are symmetric it follows that so too is \( E \), which also is defined in Lagrangian/material coordinates. The Eulerian/spatial counterpart of \( E \) is the symmetric Euler-Almansi strain tensor \( E^{EA} \) defined as,

\[
 E^{EA} = \frac{1}{2}(I - F^{-T}F^{-1}). \tag{2.15}
\]
A second order symmetric tensor, $\mathbf{A}$, may be represented by its eigenvalues, $\gamma_i$, and eigenvectors, $\mathbf{n}_i$, to form an orthonormal basis. This process is known as spectral decomposition and is determined by,

$$\mathbf{A} = \mathbf{A}\mathbf{I} = (\mathbf{A}\mathbf{n}_i) \otimes \mathbf{n}_i = \sum_{i=1}^{3} \gamma_i \mathbf{n}_i \otimes \mathbf{n}_i,$$  \hfill (2.16)

where $\otimes$ is the dyadic operator such that for two vectors $\mathbf{u}$ and $\mathbf{v}$, $(\mathbf{u} \otimes \mathbf{v})_{kj} = u_k v_j$.

Spectral decomposition is used for a number of different operations in continuum mechanics. Here it is used to determine two further strain measures, the nominal strain and the log/Hencky strain. In one dimension, the nominal strain, $\varepsilon_{\text{nom}} = (\lambda - 1)$, where $\lambda$ is the stretch ratio. In three dimensions, using (2.16), the nominal strain is,

$$\varepsilon_{\text{nom}} = \sum_{i=1}^{3} (\lambda_i - 1) \mathbf{c}_i \otimes \mathbf{c}_i$$  \hfill (2.17)

where $\lambda_i$ is the stretch ratio, which is determined from the square root of the eigenvalue of $\mathbf{C}$, and $\mathbf{c}_i$ are the eigenvectors of $\mathbf{C}$. Similarly, the log/Hencky strain in one dimension is defined as, $\varepsilon_{\text{log}} = \ln(\lambda)$. In three dimensions is is given as,

$$\varepsilon_{\text{log}} = \sum_{i=1}^{3} \ln(\lambda_i) \mathbf{c}_i \otimes \mathbf{c}_i$$  \hfill (2.18)
2.1.2.4 Rigid Body Rotations

The deformation gradient is used as the basis for measuring deformation/strain in a body. Importantly, it is insensitive to rigid body translations, i.e. rigid translation of the body will not induce deformation in the body. However, the deformation gradient is coupled with rigid body rotations. This coupling has an undesirable consequence. When a body is subjected to a rigid rotation, the deformation gradient is not equal to the identity tensor. Hence the deformation gradient now describes a deformation in the body which in reality is not there. Consequently a constitutive model will calculate a non-zero stress under rigid bdy rotation To overcome this problem, the rigid body rotation and the material deformation may be decoupled using a polar decomposition which is defined using,

\[ F = RU = vR \],

where \( R \) is the second order orthogonal rotation tensor. The tensors \( U \) and \( v \) are the right (material) stretch tensor and the left (spatial) stretch tensor respectively and both are unique, symmetric and positive-definite. They measure the stretch along their mutually orthogonal eigenvectors. The right and left stretch tensors also have the property that they are the square of the right and left Cauchy-Green deformation tensors respectively,

\[ U^2 = C \quad v^2 = b \].

In section 2.1.2.3 it was demonstrated that a tensor may be spectrally decomposed in terms of its eigenvalues and eigenvectors. Using Equation 2.16 \( U \) and \( v \) may be spectrally decomposed. The eigenvalues of the stretch tensor are the princi-
pal stretches $\lambda_a$ of the deformation and the eigenvectors are a mutually orthogonal set of unit vectors indicating the direction of the principal stretches. As the stretch tensors cannot immediately be computed from the deformation gradient. We make use of the relationships in Equation 2.20 to determine $U$ and $v$.

$$U = C^{1/2} = \sum_{a=1}^{3} \lambda_a \hat{c}^{(a)} \otimes \hat{c}^{(a)},$$  \hspace{1cm} (2.21)

$$v = b^{1/2} = \sum_{a=1}^{3} \lambda_a \hat{b}^{(a)} \otimes \hat{b}^{(a)},$$  \hspace{1cm} (2.22)

where $\hat{c}^{(a)}$ are the (normalised) eigenvectors of $C$ and $\lambda_a$ is the square root of the eigenvectors of $C$, which in fact is the principal stretch. $v$ is constructed in a similar fashion. Thus from the Cauchy–Green deformation tensors $C$ and $b$, we can compute the stretch tensors $U$ and $v$ using spectral decomposition. The rotation tensor of the polar decomposition may now be computed from a rearrangement of Equation 2.19,

$$R = FU^{-1} = v^{-1}F.$$  \hspace{1cm} (2.23)

$R$ is the rigid body rotation inherent to the deformation.

2.1.2.5 Strain Invariants

A second order tensor $A$ may be written in terms of a set of normalized eigenvectors $n_i$ with corresponding eigenvalues $\gamma_i$ such that,

$$An_i = \gamma_in_i \quad (i = 1, 2, 3; \text{ with no summation}).$$  \hspace{1cm} (2.24)
Three invariants may be computed from the eigenvalue equation given in 2.24. For the eigenvectors \( \mathbf{n}_i \) to be physical, they must comply with the criteria \( \mathbf{n}_i \neq \mathbf{0} \) and hence,

\[
\det(\mathbf{A} - \gamma_i \mathbf{I}) = 0,
\]

(2.25)

where,

\[
\det(\mathbf{A} - \gamma_i \mathbf{I}) = -\gamma_i^3 + I_1 \gamma_i^2 - I_2 \gamma_i + I_3.
\]

(2.26)

This is a cubic equation in \( \gamma \) known as the characteristic polynomial for \( \mathbf{A} \). \( I_i \) are the principal scalar invariants of \( \mathbf{A} \) and may be solved from the above equation to give,

\[
I_1(\mathbf{A}) = \text{tr} \mathbf{A} = \gamma_1 + \gamma_2 + \gamma_3
\]

\[
I_2(\mathbf{A}) = \frac{1}{2}[(\text{tr} \mathbf{A})^2 - \text{tr}(\mathbf{A}^2)] = \gamma_1 \gamma_2 + \gamma_1 \gamma_3 + \gamma_2 \gamma_3
\]

(2.27)

\[
I_3(\mathbf{A}) = \det(\mathbf{A}) = \gamma_1 \gamma_2 \gamma_3.
\]

Theses invariants are used as frame-invariant scalar measures to quantify the strain in a body. These scalar measures are known as strain invariants and are derived from the Cauchy-Green deformation tensors and are defined as follows,
\[ I_1 = \text{tr}(C) = \lambda_1 + \lambda_2 + \lambda_3 \quad (2.28) \]
\[ I_2 = \frac{1}{2} \left[ \text{tr}(C)^2 - \text{tr}(C^2) \right] = \lambda_1^2 \lambda_2 + \lambda_1^2 \lambda_3 + \lambda_2^2 \lambda_3 \quad (2.29) \]
\[ I_3 = \det(C) = J^2 = \lambda_1 \lambda_2 \lambda_3 \quad (2.30) \]

These invariants are commonly used to define the strain-energy density functions for hyperelastic materials.

### 2.1.2.6 Push-forward, Pull-back Operations

Tensors and vectors may be described in both the undeformed/Lagrangian and deformed/Eulerian configurations. A tensor or vector described in one reference frame may be mapped to the other using a push-back or pull-forward operation. For example the Green–Lagrange strain \( E \) may be mapped to the Euler-Almansi strain \( e \) via a push-forward operation or mapping, denoted as \( \chi_s(\bullet) \). In this case the operation is as follows,

\[ e = \ F^{-T} E F^{-1} = \chi_s(E) \quad (2.31) \]

In other words, a push-forward of \( E \) results in \( e \). A pull-back is the inverse operation and is denoted as \( \chi_s^{-1}(\bullet) \) and would map \( e \) to \( E \).

An important distinction exists for push-forward and pull-back operations on tensors, that is whether the tensor being operated upon is covariant or contravariant. This is a complex topic which could be discussed in detail by itself. Suffice to say that a tensor is co- or contra-variant depending on the basis vectors used to describe
its components. Generally speaking, deformation and strain tensors are covariant and stress tensors are contravariant. This is important, as the push-forward, pull-back operations differ depending on this criteria. For a covariant second order tensor the push-forward and pull-back operations are,

\[
\chi^\ast (\mathbf{\bullet})^\flat = \mathbf{F}^{-
abla}_{\mathbf{T}} (\mathbf{\bullet})^\flat \mathbf{F}^{-1}, \quad \chi^{-1\ast} (\mathbf{\bullet})^\flat = \mathbf{F}^\nabla_{\mathbf{T}} (\mathbf{\bullet})^\flat \mathbf{F},
\]

and for a contravariant second order tensor they are,

\[
\chi^\ast (\mathbf{\bullet})^\sharp = \mathbf{F} (\mathbf{\bullet})^\sharp \mathbf{F}^\nabla_{\mathbf{T}}, \quad \chi^{-1\ast} (\mathbf{\bullet})^\sharp = \mathbf{F}^{-1} (\mathbf{\bullet})^\sharp \mathbf{F}^{-\nabla}_{\mathbf{T}}.
\]

These operations are important for converting tensors which may be easily calculated in one configuration, to the configuration in which we are working. They become even more useful when multiple configurations are used, e.g. finite deformation elasto-plasticity.

2.1.2.7 Deformation Decomposition in Plasticity

The Eulerian velocity gradient is defined as \( \mathbf{L} = \nabla_{\mathbf{x}} \). In terms of the deformation gradient

\[
\mathbf{L} = \mathbf{\dot{F}F}^{-1}
\]

where \( \mathbf{\dot{F}} = \nabla_{\mathbf{t}} \mathbf{F} \). The deformation gradient may be multiplicatively split into elastic and plastic components

\[
\mathbf{F} = \mathbf{F}^\varepsilon \mathbf{F}^\varepsilon.
\]
To determine the velocity gradient in this case, the product rule is used to determine \( \dot{F} \), as is the property \( F^{-1} = F^{p-1}F^{e-1} \).

\[
L = (F^e \dot{F}^p + F^{p} \dot{F}^e)(F^{p-1}F^{e-1})
\]

\[
= F^e F^{e-1} + F^e(\dot{F}^p F^{p-1})F^{e-1}.
\]

(2.36)

The intermediate configuration prescribed by plastic deformation is not unique, both the elastic and plastic deformation gradients may consist of a rigid rotation and a stretch (via polar decomposition). To overcome this issue, in the macro-level finite deformation elasto-plastic constitutive model presented in Chapter 6 all rigid rotations are lumped into the plastic deformation gradient. Consequently, \( F^e = V^e \), and \( F^p = V^p R \). Using this assumption and the additive decomposition of \( L \) into its symmetric and skew-symmetric parts we obtain,

\[
L = L^e + V^e L^p V^{e-1}
\]

(2.37)

\[
L = L^e + V^e L^p V^{e-1}
\]

(2.38)

\[
= D^e + W^e + V^e D^p V^{e-1} + V^e W^p V^{e-1}
\]

If \( D = \text{sym}(L) \) and \( W = \text{asym}(L) \) then,

\[
D = D^e + \text{sym}(V^e D^p V^{e-1}) + \text{sym}(V^e W^p V^{e-1})
\]

(2.39)
and

\[ W = W^e + \text{asym}(V^e D^p V^{e-1}) + \text{asym}(V^e W^p V^{e-1}) \]  \hspace{1cm} (2.40)

We see that in general the deformation rate tensor cannot be additively split into elastic and plastic parts, \( D \neq D^e + D^p \). However in the case where elastic strains are small then \( V^e = V^{e-1} \approx I \), leading to \( \text{sym}(V^e D^p V^{e-1}) = D^p \) and \( \text{asym}(V^e W^p V^{e-1}) = 0 \). So, for the case of small elastic strains

\[ D = D^e + D^p \]  \hspace{1cm} (2.41)

and

\[ W = W^e + W^p \]  \hspace{1cm} (2.42)

The result from (2.41) is commonly used in finite element codes to determine strain in a step by integration of \( D \) with respect to time. It should be emphasised that correct use of (2.41) requires that elastic strains are small (Dunne and Petrinic, 2005).
2.1.3 Stress

If one imagines taking a section through a body in the current configuration (Figure 2.2), the body has a traction vector $t$ derived from the surface forces, and a vector $n$ normal to the surface of the section. The Cauchy stress $\sigma$ is a second order symmetric tensor of the force per unit deformed surface area $ds$, and is defined as,

$$ t = \sigma n. $$

(2.43)
The stress may be computed in the reference configuration too. In this case,

\[ t_0 = P n_0. \]  \hspace{1cm} (2.44)

where \( t_0 \) and \( n_0 \) are the traction and surface normal mapped back to the reference configuration. In this case, the stress is the First Piola-Kirchhoff (PK1) stress \( P \) which is the force per unit undeformed area. This measure is sometimes used for mathematical or experimental convenience, however PK1 stress is not a symmetric tensor. Depending on convention, the nominal stress \( \tilde{\sigma} \) may be defined as either the PK1 stress or its transpose. In this thesis \( \tilde{\sigma} = P \). To map the Cauchy stress in the deformed configuration to PK1 in the reference configuration, Nanson’s formula is used with the result that,

\[ \sigma = J^{-1}PF^T. \]  \hspace{1cm} (2.45)

There are a number of alternative stress tensors which are used in non-linear solid mechanics. The Kirchhoff stress \( \tau \) is based on the Cauchy stress and is simply defined as,

\[ \tau = J \sigma. \]  \hspace{1cm} (2.46)

It will be seen in a later section that the Kirchhoff stress is used in the definition of the consistent tangent matrix, a vital component in the solution of implicit finite element problems. Next, the second Piola-Kirchhoff (PK2) stress \( S \) is closely related to PK1 but is a symmetric tensor. It is based in the material (Lagrangian) coordinate system and therefore it is often used for the composition of constitutive models as
discussed in Section 2.3. The PK2 stress may expressed in terms of PK1 or the Cauchy stress as follows,

\[ S = P F^T; \quad S = J F^{-1} \sigma F^{-T}. \]

Looking at the pull-back operation for contravariant second order tensors \( \chi^{-1} (\bullet) \) in 2.33, and at 2.46, it is apparent that PK2 is a pull-back of the Kirchhoff stress \( \tau \).

Another stress tensor, the Mandel stress \( \Sigma \) is commonly used to describe inelastic materials. It is generally not symmetric and is defined as,

\[ \Sigma = C S, \]

where \( C \) is the left Cauchy-Green deformation tensor.
2.2 Finite Element Method

While some continuum mechanics problems may be solved using analytically, the solution of the majority of engineering problems require numerical techniques. Finite Element Analysis (FEA) is one such technique and it has been used throughout the studies in subsequent chapters. A commercial FE code, Abaqus (DS SIMULIA, R.I. USA), is used for the solution of FEA problems. The advantages of using a commercial code (as opposed to a custom code) include robust meshing techniques, robust solution methods and portability to name but a few. A user may customize Abaqus through a number of user-defined Fortran subroutines.

The FE method discretizes a body into a number of volumes or elements, which are interconnected at the nodes (the vertices of the element). The prescribed boundary conditions are applied to the body, and through the solution of a set of governing equations, the displacements are interpolated throughout the body based on discrete values at the element values.

2.2.1 Lagrangian Finite Element Equations

In solid mechanics, a Lagrangian description of motion is most commonly used. This is where the nodes and elements move as the material deforms. Within a Lagrangian description, one may use a updated or a total Lagrangian formulation. The work presented in this thesis uses an updated Lagrangian formulation; this is where derivatives are calculated with respect to the spatial/Eulerian coordinates and the weak form of the governing equations are computed with respect to the current/deformed configuration.

Figures 2.3 and 2.4 are schematics outlining the general procedure for the solution of the finite element equations.
Figure 2.3: Flowchart outlining the major steps for an algorithm to solve the non-linear finite element equations. Where $K_{gl}$ and $F_{gl}$ are the global stiffness and internal force arrays, respectively, $K_{el}$ and $F_{el}$ are the element stiffness and internal force arrays, respectively, $G_{gl}$ is the global residual force array, $U$ is the displacement array, $\Delta U$ is the increment of displacement for an iteration $k$. 

Yes

No

\[|G_{gl}| < \text{tol} \]

Store $U, F$ and $\varepsilon, \sigma$

\[\text{step: current increment} \]
\[\text{nstep: total number of steps} \]
\[k: \text{current iteration} \]
\[\text{niter: max. number of Newton-Raphson iterations} \]
2.2.2 Solution of the Non-Linear Finite Element Equations

The majority of problems in contemporary FE analysis involve the solution of non-linear problems. In solid mechanics there are a number of factors which may introduce non-linearity to the FE equations.

1. The strain-displacement relationship becomes non-linear. This is tantamount to the “small strain” assumption becoming invalid.

2. The stress-strain relationship is non-linear. This is common in biological tissues and elastomers. Plasticity too results in a non-linear stress-strain relationship.

3. Large displacements (though not necessarily large strains) result in non-linear FE equations.

4. Discontinuities such as contact or fracture induce non-linearities and may require further treatment than methods mentioned here to attain a solution.

Generally, the finite element equations are based upon the principal of virtual work. The Updated Lagrangian (UL) FE equations used in this thesis are based on an extension of this, the principal of virtual displacement. This formulation is given in the current configuration as,

\[ \int_V \sigma_{ij} \delta e_{ij} = \mathfrak{R}, \]  

where we wish to solve (2.49) at a time \( t + \Delta t \), \( \sigma_{ij} \) is the Cauchy stress, \( e_{ij} \) is the linear strain tensor defined as, \( e_{ij} = \frac{1}{2} (u_{i,j} + u_{j,i}) \), \( V \) is the current volume, \( \delta \) is the variational operator. The external virtual work \( \mathfrak{R} \) is the externally applied work.
due to surface tractions and body forces at time $t + \Delta t$,

$$
\mathcal{R} = \int_V f^B_i \delta u_i dV + \int_S f^S_i \delta u_i dS,
$$

(2.50)

where $f^B_i$ and $f^S_i$ are the externally applied body and surface force vectors respectively, and $\delta u_i$ is the variational displacement vector, $V$ and $S$ are the volume and surface areas over which the external forces are applied.

We wish to solve (2.49) at time $t + \Delta t$, however there is insufficient information to do so. Using the principal of work conjugacy, (2.49) may be written using quantities at time $t$,

$$
\int_V \left. \int_t^{t+\Delta t} \sigma_{ij} \delta_{ij} E_{ij} \right|_t^{t+\Delta t} d^tV = \mathcal{R}.
$$

(2.51)

The convention in this equation (adopted from Bathe (2006)) is that a left superscript indicates the time at which a quantity occurs and a left subscript indicates the time with respect to which the quantity is measured, where $S_{ij}$ is the second Piola–Kirchhoff stress, $E_{ij}$ is the Green–Lagrange strain, and $^tV$ the volume at time $t$.

The 2PK stress may be decomposed as,

$$
\left. t^{+\Delta t} S_{ij} \right|_t = \left. tS_{ij} \right|_t + \left. t\sigma_{ij} \right|_t + \left. tS_{ij} \right|_t
$$

(2.52)

where $\sigma_{ij}$ is the known Cauchy stress at time $t$, and $S_{ij}$ is the unknown increment of stress from time $t$ to time $t + \Delta t$. The variational of the strain may be decomposed
similarly,

$$\delta^{t+\Delta t} E_{ij} = \delta^t E_{ij} + \delta_t E_{ij} = \delta_t E_{ij}$$  \hspace{1cm} (2.53)$$

where the variational of strain at time $t$ w.r.t. time $t$ is zero, and we are left with the variational of the increment of strain $\delta_t E_{ij}$. The Green-Lagrange strain written in terms of displacements is given as,

$$E_{ij} = \frac{1}{2} (u_{i,j} + u_{j,i} + u_{k,i} u_{k,j}),$$  \hspace{1cm} (2.54)$$

which may be split into linear and non-linear parts. Hence (2.53) is written as,

$$\epsilon_t E_{ij} = \epsilon_e E_{ij} + \epsilon_h E_{ij}; \hspace{0.5cm} \delta_t E_{ij} = \delta E_e E_{ij} + \delta E_h E_{ij};$$  \hspace{1cm} (2.55)$$

where $\epsilon_e E_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i})$ and $\epsilon_h E_{ij} = \frac{1}{2}(u_{k,i} u_{k,j})$. Using (2.52), (2.53) and (2.55), (2.51) may be rewritten as,

$$\int_{V}^{} t S_{ij} \delta_t E_{ij} d^t V + \int_{V}^{} t \sigma_{ij} \delta \eta_{ij} d^t V = t^{+\Delta t} \mathbf{R} - \int_{V}^{} t \sigma_{ij} \delta \epsilon_{ij} d^t V.$$  \hspace{1cm} (2.56)$$

Equation (2.56) is a complex non-linear function of the unknown displacement increment. It is necessary to linearise (2.56) to enable us to compute a solution. The linearisation assumes the matrix form,

$$^{t} \mathbf{K} \mathbf{U} = t^{+\Delta t} \mathbf{R} - ^{t} \mathbf{F};$$  \hspace{1cm} (2.57)$$
where $\mathbf{K}$ is the incremental stiffness matrix, $\mathbf{U}$ is the vector of increments in nodal point displacements, $\mathbf{R}^{t+\Delta t}$ is the vector of externally applied nodal forces at time $t + \Delta t$, and $\mathbf{F}$ is the vector of nodal point forces equivalent to the element stresses at time $t$.

Each of the terms in (2.56) are individually assessed for linearity in the unknown displacement $u_i$. The first term on the left hand side of (2.56) contains both linear and higher order terms in $u_i$. In general, the stress step $\delta E_{ij}$ is a non-linear function of $\epsilon_{ij}$. The variational of the strain step $\delta E_{ij}$ is a linear function of $u_i$. The stress step may be expressed as a Taylor series where the higher order terms are neglected,

$$\delta S_{ij} = \frac{\partial S_{ij}}{\partial E_{rs}} \epsilon_{rs} + \text{H.O. Terms}.$$  \hspace{1cm} (2.58)

Using the decomposition of the Green–Lagrange strain presented in (2.55), (2.58) may be rewritten as,

$$\delta S_{ij} = \frac{\partial S_{ij}}{\partial E_{rs}} (\epsilon_{rs} + \eta_{rs}) = tC_{ijrs} \epsilon_{rs}.$$  \hspace{1cm} (2.59)

As $\eta_{rs}$ is quadratic in $u_i$ it is neglected and all that remains is a linearised term for the stress step, where $tC_{ijrs}$ is the incremental tangent matrix describing stress-strain behaviour. Using this linearisation, the first term of (2.56) is rewritten as,

$$\int_{\Omega} tS_{ij} \delta \epsilon_{ij} \, d^4V \approx \int_{\Omega} tC_{ijrs} \epsilon_{rs} \delta \epsilon_{ij} \, d^4V$$  \hspace{1cm} (2.60)
The second term of (2.56) is assessed next for linearity in $u_i$. The Cauchy stress $^tS_{ij}$ is not a function of $u_i$. The variational of the non-linear strain step $^t\eta_{ij}$ is linear in $u_i$. This means that no amendment is required for the second term on the left side of (2.56), nor is it required to change the second term on the right side of (2.56). The linearised form of (2.56) is given as,

$$
\int_V i_{ijrs} i_{te} \delta_{te} i_{ij} \, d^tV + \int_V i_{\sigma ij} \delta_{t\eta ij} \, d^tV = t^{+\Delta t} R - \int_V i_{\sigma ij} \delta_{te} i_{ij} \, d^tV \tag{2.61}
$$

This linearised equation is discretized using the shape functions outlined in Section 2.2.3;

$$
\int_V i_{C_{ijrs} i_{te} \delta_{te} i_{ij} \, d^tV = \delta U^T \left( \int_V i_{B_L} i_C i_{B_L} \, d^tV \right) = \delta U^T (iK_L U) \\
\int_V i_{\sigma ij} \delta_{t\eta ij} \, d^tV = \delta U^T \left( \int_V i_{B_{NL}} i_{\tilde{\sigma}} i_{B_{NL}} \, d^tV \right) = \delta U^T (iK_{NL} U) \\
\int_V i_{\sigma ij} \delta_{te} i_{ij} \, d^tV = \delta U^T \left( \int_V i_{B_L} i_{\tilde{\sigma}} \, d^tV \right) = \delta U^T (iF) \\
^{t+\Delta t} R = \delta U^T (t^{+\Delta t} R)
$$

where $B_L$ is a matrix of linear shape function derivatives, $C$ is the material tangent matrix, $B_{NL}$ is a matrix of higher order shape function derivatives, $\tilde{\sigma}$ is a matrix of Cauchy stress components, $\tilde{\sigma}$ is the Cauchy stress in Voigt (vector) notation, $K_L$ is the linear incremental stiffness matrix, and $K_{NL}$ is the non-linear incremental stiffness matrix. The linearised matrix equation (2.57) can now be cast in the updated Lagrangian formulation using (2.62). It is important to note that this is a linearised equation which in itself will not calculate the configuration at time $t + \Delta t$.

A Newton-Raphson scheme is typically used to iteratively solve for the configuration at time $t + \Delta t$ (see Section 2.2.4 for details on Newton-Raphson method). The basic equation to be solved is (2.49). In its discretized form, it is expressed in
terms of forces,

\[ t + \Delta t \mathbf{R} - t + \Delta t \mathbf{F} = 0 \]  

(2.63)

where \( t + \Delta t \mathbf{R} \) is a vector of the externally applied nodal forces at time \( t + \Delta t \), \( t + \Delta t \mathbf{F} \) is a vector of the internal node forces at time \( t + \Delta t \) that are equivalent to the element stresses. In a Newton-Raphson iteration where \( k = 1, 2, 3, \ldots \)

\[- \mathbf{G}^{(k-1)} = t + \Delta t \mathbf{R} - t + \Delta t \mathbf{F}^{(k-1)} \]  

(2.64)

where \( \mathbf{G}^{(k-1)} \) is an residual force vector. The incremental improvement in the calculated nodal displacement \( \Delta \mathbf{U}^{(k)} \) for iteration \( k \) is computed using the linearised equations presented in (2.61) and (2.62),

\[(\mathbf{K}_L + \mathbf{K}_{NL})^{(k-1)} \Delta \mathbf{U}^{(k)} = -\mathbf{G}^{(k-1)}, \]  

(2.65)

where \( \mathbf{K} = \mathbf{K}_L + \mathbf{K}_{NL} \). Using (2.65) the nodal displacements are updated for each increment \( k \) using,

\[ t + \Delta t \mathbf{U}^{(k)} = t + \Delta t \mathbf{U}^{(k-1)} + \Delta \mathbf{U}^{(k)}, \]  

(2.66)

where for the initial increment \( k = 1 \), \( t + \Delta t \mathbf{U}^{(0)} = \mathbf{U} \) and \( t + \Delta t \mathbf{F}^{(0)} = \mathbf{F} \). Equations (2.65) and (2.66) are continuously solved until a convergence criterion is met. For example if the norm of the residual force vector, \( ||\mathbf{G}|| < \text{tol} \), where \( \text{tol} \) is some predefined scalar tolerance value on the order of \( 10^{-3} \) to \( 10^{-6} \).
Finally, the integrals in (2.62) are evaluated using Gaussian quadrature, which is outlined in Section 2.2.3. These updated Lagrangian finite element equations can be solved using an algorithm that is based on the flowchart given in Figure 2.3.

### 2.2.3 Finite Element Discretization

One of the key aspects of the finite element method is the use of shape functions to interpolate both coordinates and displacements of the nodes in a finite element mesh. For displacements, this can neatly be summarised as follows,

$$u_i(x) = \sum_{a=1}^{npel} N_a(x) u_{ia}, \quad (2.67)$$

where \(x\) and \(u\) are the coordinates and displacement of the node in question, \(N_a(x)\) is the shape function for the node \(a\) evaluated at \(x\), and \(npel\) is the number of nodes per element.

### 2.2.3.1 Shape Function Derivatives

The solution of the finite element equations requires the evaluation of the derivatives of shape functions with respect to the model coordinate system. Shape functions are typically written with respect to a parent coordinate system. A Jacobian mapping is used to determine the derivatives with respect to model coordinates by utilising the derivatives with respect to the parent coordinates, \(r\) and \(s\), as follows. In 2D,

$$\begin{bmatrix} \frac{\partial N_a}{\partial r} \\ \frac{\partial N_a}{\partial s} \end{bmatrix} = \begin{bmatrix} \frac{\partial x_1}{\partial r} & \frac{\partial x_2}{\partial r} \\ \frac{\partial x_1}{\partial s} & \frac{\partial x_2}{\partial s} \end{bmatrix} \begin{bmatrix} \frac{\partial N_a}{\partial x_1} \\ \frac{\partial N_a}{\partial x_2} \end{bmatrix}, \quad (2.68)$$
where,

\[
J = \begin{bmatrix}
\frac{\partial x_1}{\partial r} & \frac{\partial x_2}{\partial r} \\
\frac{\partial x_1}{\partial s} & \frac{\partial x_2}{\partial s}
\end{bmatrix},
\]

is the Jacobian matrix. The desired derivatives of the shape functions are found using the inverse relationship,

\[
\begin{bmatrix}
\frac{\partial N_a}{\partial x_1} \\
\frac{\partial N_a}{\partial x_2}
\end{bmatrix} = J^{-1} \begin{bmatrix}
\frac{\partial N_a}{\partial r} \\
\frac{\partial N_a}{\partial s}
\end{bmatrix}.
\]

(2.69)

The determinant of the Jacobian matrix, \(|J|\) is another important measure for the calculation of the finite element equations as it relates the model space element volume to the parent space volume \(dV = |J| dV_{PS}\).

### 2.2.3.2 Integration using Gaussian Quadrature

Gaussian quadrature is an effective numerical scheme for approximating the definite integral of a function, without having to compute the integral itself. Instead the function is evaluated at a number of integration points (Gauss points) and the weighted sum of the sample points is the definite integral of the function. In one dimension this is expressed as,

\[
\int_{-1}^{1} f(\xi) d\xi \approx \sum_{i=1}^{n} w_i f(\xi_i),
\]

(2.70)

where \(f(\xi)\) is a function of the variable \(\xi\), \(w_i\) is the Gauss weight, \(\xi_i\) is the Gauss point, and \(n\) is the number of Gauss points. This concept may be extended to two
Chapter 2

Assemble Global Arrays
The global arrays are formed by summing the element arrays, using the connectivity array to ensure that the element-level components are placed correctly in the global array

\[ K_{gL}^{el} = \sum_{el=1}^{nelm} K_{gL}^{el}, \quad K_{nL}^{el} = \sum_{el=1}^{nelm} K_{nL}^{el}, \quad F_{gL} = \sum_{el=1}^{nelm} F^{el} \]

Connectivity array
\[ u_{el} \Leftrightarrow u_{gL} \]

Calculate Element Arrays
The element arrays are computed by summing the quantities below over each integration point.

\[ K_{gL}^{el} = \sum_{p=1}^{nint} W_p (B [\epsilon_B L J] )_p, \quad K_{nL}^{el} = \sum_{p=1}^{nint} W_p (B_NL [\sigma_B J] )_p, \quad F^{el} = \sum_{p=1}^{nint} W_p (B [\sigma J] )_p \]

Integrate Point Level

Int. Point Coordinate: \((r,s,t)\)
Element Coordinates: \((x_1, x_2, x_3)\)

Calculate shape functions, shape function gradients and Jacobian determinant at the integration point

Form the \(B_L\) and \(B_{NL}\) matrices

Calculate the strain \(\epsilon\)

Calculate the stress \(\sigma\) and tangent matrix \(\mathbb{C}\)

Figure 2.4: Schematic showing how calculations for stress and strain at the integration point level feed up to the element level, for integration using Gaussian quadrature. The element level arrays are then fed up to the global level via the connectivity array. The global level arrays are then solved using (2.65) to solve for the displacement.
dimensions,

$$\int_{-1}^{1} \int_{-1}^{1} f(\xi, \eta) d\xi d\eta \approx \sum_{i=1}^{n} w_i f(\xi_i, \eta_i), \quad (2.71)$$

and three dimensions,

$$\int_{-1}^{1} \int_{-1}^{1} \int_{-1}^{1} f(\xi, \eta, \zeta) d\xi d\eta d\zeta \approx \sum_{i=1}^{n} w_i f(\xi_i, \eta_i, \zeta_i). \quad (2.72)$$

Gaussian quadrature is remarkably accurate given its simplicity and facilitates the quick solution of integrals. This method allows for the straightforward evaluation of the integrals in (2.62) resulting in (2.65).

### 2.2.3.3 Incorporation into the Finite Element Equations

Figure 2.4 gives a schematic showing how the array of shape function derivatives $B$, the stress $\sigma$, and the tangent matrix $C$, which are calculated at the integration/Gauss points are used to calculate the element level stiffness matrices $K^l_{el}$ and $K^d_{el}$, and the nodal forces $F^l_{el}$. These then are fed into the global stiffness and nodal force matrices, $K^l_{gl}$, $K^d_{gl}$, and $F^l_{gl}$, via a connectivity array. These global arrays are then used to solve the finite element equations given in (2.65).
2.2.4 Newton-Raphson Method in Multiple Variables

Newton’s method is a mathematical procedure commonly used to determine the root of a function, \( f(x) = 0 \). It is used to implicitly solve non-linear FE problems presented in Section 2.2.3. In the current research it is also used in the implicit algorithmic implementation of plasticity constitutive models. This method first linearises the function, \( f(x) \), then using an initial guess \( x_0 \) the root of the function is iteratively determined. Subsequent values of \( x \) are determined using the following formula,

\[
x_{n+1} = x_n - J^{-1}_{x_n} f(x_n),
\]

where \( J^{-1}_{x_n} \) is the Jacobian matrix of \( f(x) \) at the given \( x_n \), where \( J_{ij} = f_{i,j} \) (\( f_{i,j} \) is the derivative of \( f(x_i) \) with respect to \( j \)). The correct value of \( x \) is adjudged to have been converged upon when \( \| f(x_n) \| < f_{tol} \) where \( f_{tol} \) is typically on the order of \( 10^{-3} \) to \( 10^{-6} \).

Newton’s method has the property of quadratic convergence and hence is an efficient algorithm to determine the root of a function. The one drawback to using this method is that \( f(x) \) must be differentiable with respect to \( x \).

2.2.5 Explicit Solution of the Finite Element Equations

Though no simulations in this thesis are solved using the explicit method, a brief discussion of the topic is presented here for completeness. Again, Equation (2.49) must be solved. Its discretised equivalent is,

\[
\delta U^T \left( \int_V t \mathbf{B}_L^T \mathbf{\sigma} \, dV \right) - \delta U^T (\mathbf{\Gamma}) = 0
\]
and the residual force vector $G$ (dropping the superscripts and the variational of the displacement) is,

$$\int_V B_L^T \sigma \, dV - R = G = 0. \quad (2.75)$$

To solve for the state at $t + \Delta t$, a stiffness matrix based on the solution at time $t$, $K'$, is calculated. The incremental nodal displacements are then solved directly using this stiffness matrix and the increment in external nodal forces,

$$K' \Delta U = \Delta R. \quad (2.76)$$

This calculation is performed only once, there is no iteration or checks for convergence. The accuracy of the method is dependent on an increment being quasi-linear. Therefore one must use multiple times more time steps for an explicit analysis compared to an implicit analysis.
2.3 Constitutive Laws

2.3.1 Linear Elasticity

The theory of linear elasticity stems from the early experiments of Robert Hooke who stated “ut tensio, sic vis” (as the extension, so the force). That is to say that the force $F$ required to extend a filament by a displacement $u$ is proportional to that displacement, i.e. $F = ku$, where $k$ is the constant of proportionality known as the stiffness.

Hooke’s law is normalised by using stress and strain, rather than force and displacement. In the linear elasticity regime it is assumed that strains are small (infinitesimal), such that the previously defined Green-Lagrange, Euler-Almansi and nominal strain tensors are approximately equal to the infinitesimal strain tensor $\varepsilon$. Similarly the nominal and Cauchy stress are assumed to be equivalent, for simplicity the stress tensor is referred to as $\sigma$. The constant ratio of the stress to strain defines the Young’s modulus of the material.

To extended this law to three dimensions, lateral deformations must be included. When an isotropic material is extended axially in uniaxial tension, a lateral contraction typically occurs and is proportional to the axial strain. This is known as the Poisson’s effect and the ratio of lateral strain $\varepsilon_{ii}$ to axial strain $\varepsilon_{jj}$ is the Poisson’s ratio $\nu = -\varepsilon_{ii}/\varepsilon_{jj}$.

$$
\begin{align*}
\varepsilon_{11} &= \frac{1}{E}(\sigma_{11} - \nu(\sigma_{22} + \sigma_{33})) \\
\varepsilon_{22} &= \frac{1}{E}(\sigma_{22} - \nu(\sigma_{11} + \sigma_{33})) \\
\varepsilon_{33} &= \frac{1}{E}(\sigma_{33} - \nu(\sigma_{11} + \sigma_{22}))
\end{align*}
$$ (2.77)
and the shear stress-strain behaviour is defined using the shear modulus $\mu$.

$$
\varepsilon_{12} = \frac{1}{(2 \mu)} \sigma_{12} \\
\varepsilon_{13} = \frac{1}{(2 \mu)} \sigma_{13} \\
\varepsilon_{23} = \frac{1}{(2 \mu)} \sigma_{23}
$$

Equation (2.77) be written in index notation as $\varepsilon_{ij} = D_{ijkl} \sigma_{kl}$ where $D_{ijkl}$ is the fourth order compliance tensor. The inverse of (2.77) can be used to determine the stress given strain, $\sigma_{ij} = C_{ijkl} \varepsilon_{kl}$ where $C = D^{-1}$ is the stiffness tensor. Due to major and minor symmetries of the stiffness/compliance tensor it may be presented in Voigt notation as a $6 \times 6$ matrix, with the stress and strain tensors written in vector form.

$$
\begin{bmatrix}
\sigma_{11} \\
\sigma_{22} \\
\sigma_{33} \\
\sigma_{12} \\
\sigma_{13} \\
\sigma_{23}
\end{bmatrix}
= \frac{E}{(1 + \nu)(1 - 2\nu)}
\begin{bmatrix}
1 - \nu & \nu & \nu & 0 & 0 & 0 \\
\nu & 1 - \nu & \nu & 0 & 0 & 0 \\
\nu & \nu & 1 - \nu & 0 & 0 & 0 \\
0 & 0 & 0 & \mu & 0 & 0 \\
0 & 0 & 0 & 0 & \mu & 0 \\
0 & 0 & 0 & 0 & 0 & \mu
\end{bmatrix}
\begin{bmatrix}
\varepsilon_{11} \\
\varepsilon_{22} \\
\varepsilon_{33} \\
2\varepsilon_{12} \\
2\varepsilon_{13} \\
2\varepsilon_{23}
\end{bmatrix}
$$

2.3.2 Hyperelasticity

A hyperelastic material is a specific class of material for which the constitutive equation is derived from a Helmholtz strain-energy potential $\Psi$. It is particularly useful for the development of constitutive models concerned with finite strains. This section gives a brief outline of the derivation of various stress from the Helmholtz strain-energy $\Psi$. 
2.3.2.1 Stress Derivation

The Lagrangian configuration, the second Piola-Kirchhoff stress defined by the derivative of $\Psi$ either with respect to the right Cauchy-Green deformation tensor, $C$, or the Green-Lagrange strain tensor, $E$, as,

$$S = 2 \frac{\partial \Psi(C)}{\partial C} = \frac{\partial \Psi(E)}{\partial E}$$  \hspace{1cm} (2.80)

a push-forward of the second Piola-Kirchhoff stress from the material configuration to the spatial configuration will result in the Cauchy stress. Alternatively the strain-energy potential may be phrased in terms of the left Cauchy-Green deformation tensor $b$, and hence no push-forward operation is required.

$$\sigma = 2J^{-1}F \frac{\partial \Psi(C)}{\partial C} F^T = 2J^{-1}b \frac{\partial \Psi(b)}{\partial b}$$  \hspace{1cm} (2.81)

Strain energy potentials are often phrased in terms of strain invariants (see Section 2.1.2) where $\Psi(C) = \Psi(I_1, I_2, I_3)$. For isotropic strain-energy potentials, the derivative of $\Psi$ with respect to $C$ can be determined using the chain rule,

$$\frac{\partial \Psi(C)}{\partial C} = \frac{\partial \Psi}{\partial I_1} \frac{\partial I_1}{\partial C} + \frac{\partial \Psi}{\partial I_2} \frac{\partial I_2}{\partial C} + \frac{\partial \Psi}{\partial I_3} \frac{\partial I_3}{\partial C}$$  \hspace{1cm} (2.82)

to solve the above equation it is necessary to determine the derivatives of the invariants with respect to the right Cauchy-Green tensor $C$.

$$\frac{\partial I_1}{\partial C} = I, \quad \frac{\partial I_2}{\partial C} = I_1 I - C, \quad \frac{\partial I_3}{\partial C} = I_3 C^{-1}$$  \hspace{1cm} (2.83)
using these identities and inserting them back into Equation 2.82 we obtain the following expression for the second Piola-Kirchhoff stress.

\[
S = 2 \left[ \left( \frac{\partial \Psi}{\partial I_1} + I_1 \frac{\partial \Psi}{\partial I_2} \right) I - \frac{\partial \Psi}{\partial I_2} C + I_3 \frac{\partial \Psi}{\partial I_3} C^{-1} \right] \quad (2.84)
\]

through the push-forward operation in Equation 2.81, the Cauchy stress given as a function of \( b \) as,

\[
\sigma = 2 J^{-1} \left[ \left( I_2 \frac{\partial \Psi}{\partial I_2} + I_3 \frac{\partial \Psi}{\partial I_3} \right) I + \frac{\partial \Psi}{\partial I_1} b - I_3 \frac{\partial \Psi}{\partial I_2} b^{-1} \right] \quad (2.85)
\]

The Cauchy stress is the stress in the deformed configuration and hence is often the stress measure of interest.

2.3.2.2 Decoupled Strain Energy Function

To manage problems involving incompressibility, it is convenient to additively decouple the isochoric and volumetric response of the Helmholtz strain-energy potential.

\[
\Psi(C, J) = \Psi_{\text{vol}}(J) + \Psi_{\text{iso}}(C) \quad (2.86)
\]

where \( \Psi_{\text{vol}}(J) \) is the volumetric response which is solely a function of the volume change \( J \), and \( \Psi_{\text{iso}}(C) \) is the isochoric response which is a function of the isochoric right Cauchy-Green deformation tensor defined as \( C = J^{-2/3} C \). The isochoric right Cauchy-Green deformation tensor removes all volumetric contributions to the deformation.

Just as the strain-energy is additively decoupled, so too is the stress. In the
Lagrangian configuration the second Piola Kirchhoff stress is defined as,

\[ \mathbf{S} = \mathbf{S}_{\text{vol}} + \mathbf{S}_{\text{iso}} \]  

(2.87)

where \( \mathbf{S}_{\text{vol}} \) and \( \mathbf{S}_{\text{iso}} \) are the volumetric and isochoric contributions to the stress respectively, and are defined as per (2.80).

\[ \mathbf{S}_{\text{vol}} = 2 \frac{\partial \Psi_{\text{vol}}(J)}{\partial \mathbf{C}} = 2 \frac{\partial \Psi_{\text{vol}}(J)}{\partial J} \frac{\partial J}{\partial \mathbf{C}} \]  

(2.88)

\[ \mathbf{S}_{\text{iso}} = 2 \frac{\partial \Psi_{\text{iso}}(\mathbf{C})}{\partial \mathbf{C}} = 2 \frac{\partial \Psi_{\text{iso}}(\mathbf{C})}{\partial \mathbf{C}} \frac{\partial \mathbf{C}}{\partial \mathbf{C}} \]  

(2.89)

Using the following identities, explicit expressions for (2.88) and (2.89) can be determined

\[ \frac{\partial J}{\partial \mathbf{C}} = \frac{J}{2} \mathbf{C}^{-1}; \quad \frac{\partial J^{-2/3}}{\partial \mathbf{C}} = \frac{1}{3} J^{-2/3} \mathbf{C}^{-1} \]  

(2.90)

\[ \frac{\partial \mathbf{C}}{\partial \mathbf{C}} = \frac{\partial J^{-2/3} \mathbf{C}}{\partial \mathbf{C}} = J^{-2/3} \left( \mathbf{I} + J^{-2/3} \mathbf{C} \otimes \frac{\partial J^{-2/3}}{\partial \mathbf{C}} \right) \]  

\[ = J^{-2/3} \left( \mathbf{I} - J^{-2/3} \frac{1}{3} \mathbf{C} \otimes \mathbf{C}^{-1} \right) \]  

(2.91)

where \( \mathbf{I} \) is the fourth order identity matrix.

The equivalent operation for the derivation of the Cauchy stress can be per-
formed. The stress is additively decomposed,

\[ \sigma = 2J^{-1}b \frac{\partial \Psi(b)}{\partial b} = \sigma_{\text{vol}} + \sigma_{\text{iso}} \tag{2.92} \]

The specific expressions for the volumetric stress \( \sigma_{\text{vol}} \) and the isochoric stress \( \sigma_{\text{iso}} \) are given as,

\[ \sigma_{\text{vol}} = 2J^{-1}b \frac{\partial \Psi_{\text{vol}}(J)}{\partial b} = 2J^{-1}b \frac{\partial \Psi_{\text{vol}}(J)}{\partial J} \frac{\partial J}{\partial b} = \frac{\partial \Psi_{\text{vol}}(J)}{\partial J} I \tag{2.93} \]

\[ \sigma_{\text{iso}} = 2J^{-1}b \frac{\partial \Psi_{\text{iso}}(B)}{\partial b} = 2J^{-1}b J^{-2/3} \left( I - \frac{1}{3} b^{-1} \otimes b \right) : \frac{\partial \Psi_{\text{iso}}(B)}{\partial B} \]

\[ = \left( I - \frac{1}{3} b^{-1} \otimes b \right) : \sigma \tag{2.94} \]

\[ = \text{dev}(\sigma) \]

where \( \text{dev}(\bullet) \) is the deviatoric operator defined as \( \text{dev}(\bullet) = (\bullet - \frac{\text{tr}(\bullet)}{3} I) \) and the stress term \( \sigma \) is given by the expression,

\[ \sigma = 2J^{-1}b \frac{\partial \Psi_{\text{iso}}(B)}{\partial B} \tag{2.95} \]

### 2.3.2.3 Rigid Body Rotations in the Abaqus/Standard

There are a number of ways in which rigid body rotation may be dealt. When dealing with anisotropic materials, it is often necessary to assign a local material coordinate
system to an element, that rotates along with rigid body rotations, in order for directions of preferred strength to be maintained. When writing a custom material (known as a UMAT) for the Abaqus/Standard finite element analysis program, one must be aware of what coordinate system the deformation gradient used is in. A local material coordinate system can be assigned to a mesh using the *orientation keyword. In this case the deformation gradient $F'$ is computed with respect to this local coordinate system using,

$$F' = R^T FR,$$  \hspace{1cm} (2.96)

where $R$ is the rotation tensor calculated from the polar decomposition of $F'$. This operation is known as a change of basis, and it may be performed on many other tensors, for example stress tensors.

As the deformation gradient has been rotated so that it is with respect to the correct basis, no modifications to constitutive laws are required. However if one is using internal vectors/tensors that the program is not “aware” of, then these tensors must undergo a change of basis too. For example, unit vectors $a_0$ in the reference configuration are used to define directions of preferred strength in anisotropic constitutive models. These unit vectors must undergo a change of basis before they are used any further using the operation,

$$a'_0 = R^T a_0.$$  \hspace{1cm} (2.97)

### 2.3.2.4 Rigid Body Rotations in Abaqus/Explicit

In Abaqus/Explicit we are faced with a slightly different problem. In this case when writing a custom material (known as a VUMAT) the stress is based in a co-
rotational coordinate system (the same as the local coordinate system when using *orientation in a UMAT). However the deformation gradient, regardless of whether a local material frame (*orientation) is used or not, passed into the VUMAT is based in the global coordinate system.

Hyperelastic laws are commonly based on the left Cauchy-Green deformation tensor $b$. However recalling the polar decomposition it is easy to see that $b$ consists of both a deformation and a rigid body rotation. So, if $b$ were to be used, rigid body rotations would be accounted for twice as we are in a co-rotational system. To avoid this, one uses polar decomposition and bases the constitutive equation on the right stretch tensor $U$.

$$b = FF^T = (RU)(RU)^T = RU^2R^T$$ (2.98)

A general equation for a hyperelastic constitutive model is that $\sigma = \Phi(F)$. If we wish to phrase this equation in terms of the stretch tensor, we find the general equation becomes $\sigma = R\Phi(U)R^T$, where $\sigma^{\text{co-rot}} = \Phi(U)$ is the stress to be returned to the finite element software.

Examples

**Neo-Hookean**

$$\sigma = \frac{2}{J}C_{10}(\overline{b} - \frac{\text{tr}(\overline{b})}{3}I) + \frac{2}{D_1}(J-1)I$$

$$\sigma = \frac{2}{J}C_{10}(RU^2R^T - R\frac{\text{tr}(U^2)}{3}R^T)I + \frac{2}{D_1}(J-1)\text{RIR}^T$$ (2.99)

$$\sigma = R \left( \frac{2}{J}C_{10}(\overline{U}^2 - \frac{\text{tr}(\overline{U}^2)}{3}I) + \frac{2}{D_1}(J-1)I \right) R^T$$
In this case the term in the brackets is the co-rotational stress and is a function of $U$. Moving on to anisotropy, we see in (2.97) that the state variables such as vectors must be rotated to the correct reference frame. However that is not the case when working in with the stretch tensor. Here the deformation is defined in the global basis and there is not need to rotate the unit vector $a_0$.

\[
a = Fa_0 = RUa_0
\]  

(2.100)

and so the tensor (dyadic) product results in

\[
a \otimes a = aa^T = (RUa_0)(RUa_0)^T = R((Ua_0)(Ua_0)^T)R^T
\]  

(2.101)

thus when constructing constitutive models in the co-rotational basis one uses,

\[
(a \otimes a)' = (Ua_0)(Ua_0)^T
\]  

(2.102)

as the tensor product. Finally, all invariants remain, of course, the same under rigid body rotation. However they may be formulated in terms of the stretch tensors. For
instance the anisotropic invariant $I_4$, 

\[
I_4 = a_{04} \cdot C a_{04} \\
= a_{04} \cdot R^T v^2 R a_{04} \\
= a_{04} \cdot R^T RU^2 R^T R a_{04} \\
= a_{04} \cdot U^2 a_{04}
\] (2.103)
2.3.3 The Consistent Tangent Matrix

The consistent tangent matrix (CTM) is a term that is use to describe the constitutive behaviour and is used for the expedient and accurate solution of the implicit finite element equations. In infinitesimal elasticity the CTM is quite simply the stiffness matrix relating stress to strain. However in case of hyperelastic materials that undergo rigid rotations and/or finite strains the derivation of the CTM requires further thought.

The fourth order Lagrangian elasticity tensor relates the rate of the 2nd Piola Kirchhoff stress to the rate of the right Cauchy-Green deformation tensor,

\[
\dot{\mathbf{S}} = \mathbf{C} : \frac{1}{2} \dot{\mathbf{C}} \tag{2.104}
\]

\[
\mathbf{C} = 2 \frac{\partial \mathbf{S}}{\partial \mathbf{C}}; \quad C_{ijkl} = 2 \frac{\partial S_{ij}}{\partial C_{lk}} \tag{2.105}
\]

Alternatively it may be described in terms of the of the strain energy density function \(\Psi(\mathbf{C})\).

\[
\mathbf{C} = 4 \frac{\partial^2 \Psi(\mathbf{C})}{\partial \mathbf{C} \partial \mathbf{C}} \tag{2.106}
\]

In this case we are simply using the definition of the PK2 stress \(\mathbf{S}\) in an isotropic hyperelastic material. The elasticity tensor can be transformed to the Eulerian
configuration by a push-forward operation times $J^{-1}$:

$$\mathbf{c} = \chi_*(\mathbf{C}) \quad (2.107)$$

$$c_{ijkl} = J^{-1} F_{mi} F_{nj} F_{pk} F_{ql} C_{mnpq} \quad (2.108)$$

Alternatively it may be defined in terms of the Eulerian left Cauchy-Green deformation tensor $\mathbf{b}$:

$$\mathbf{c} = 4J^{-1}\mathbf{b} \frac{\partial^2 \Psi(\mathbf{b})}{\partial \mathbf{b} \partial \mathbf{b}} \mathbf{b} \quad (2.109)$$

2.3.3.1 Objective Rates

The Eulerian elasticity tensors given in (2.108) and (2.109) are given in terms of the material derivative, or Lie derivative, of the Kirchhoff stress $\tau$ (Prot et al., 2007). This is also known as the Oldroyd or Truesdell rate and is defined as:

$$\mathcal{L}(\tau) = J\mathbf{c} : \mathbf{D} \quad (2.110)$$

The Lie derivative of the Kirchhoff stress is defined as,

$$\mathcal{L}(\tau) \equiv \dot{\tau} - \mathbf{L} \tau - \tau \mathbf{L}^T = J \dot{\mathbf{\sigma}} \quad (2.111)$$
where $\dot{\sigma}$ is the Truesdell rate of the Cauchy stress, $L$ is the spatial velocity gradient defined in (2.7). Abaqus and other finite element solvers require the elasticity tensor to be defined with respect to a co-rotational rate relative to a corotated frame. Abaqus uses the Green-Naghdi rate for shell elements and the Jaumann rate for continuum elements. Using (2.111) and the additive decomposition of the velocity gradient into its symmetric and asymmetric parts, $L = D + W$, the Jaumann rate $\nabla \sigma$ of the Cauchy stress is:

$$\nabla \sigma \equiv \dot{\sigma} - W\sigma - \sigma W^T \quad (2.112)$$

and the constitutive response in the corotated frame is

$$\nabla \sigma = \nabla c : D \quad (2.113)$$

where

$$\nabla c_{ijkl} \equiv c_{ijkl} + \frac{1}{2}(\delta_{ik}\sigma_{jl} + \sigma_{ik}\delta_{jl} + \delta_{il}\sigma_{jk} + \sigma_{il}\delta_{jk}) \quad (2.114)$$
Bibliography


Chapter 3

A robust anisotropic hyperelastic formulation for the modelling of soft tissue

Abstract

The Holzapfel–Gasser–Ogden (HGO) model for anisotropic hyperelastic behaviour of collagen fibre reinforced materials was initially developed to describe the elastic properties of arterial tissue, but is now used extensively for modelling a variety of soft biological tissues. Such materials can be regarded as incompressible, and when the incompressibility condition is adopted the strain energy $\Psi$ of the HGO model is a function of one isotropic and two anisotropic deformation invariants. A compressible form (HGO-C model) is widely used in finite element simulations whereby the isotropic part of $\Psi$ is decoupled into volumetric and isochoric parts and the anisotropic part of $\Psi$ is expressed in terms of isochoric invariants. Here, by using three simple deformations (pure dilatation, pure shear and uniaxial stretch), we demonstrate that the compressible HGO-C formulation does not correctly model
compressible anisotropic material behaviour, because the anisotropic component of the model is insensitive to volumetric deformation due to the use of isochoric anisotropic invariants. In order to correctly model compressible anisotropic behaviour we present a modified anisotropic (MA) model, whereby the full anisotropic invariants are used, so that a volumetric anisotropic contribution is represented. The MA model correctly predicts an anisotropic response to hydrostatic tensile loading, whereby a sphere deforms into an ellipsoid. It also computes the correct anisotropic stress state for pure shear and uniaxial deformation. To look at more practical applications, we developed a finite element user-defined material subroutine for the simulation of stent deployment in a slightly compressible artery. Significantly higher stress triaxiality and arterial compliance are computed when the full anisotropic invariants are used (MA model) instead of the isochoric form (HGO-C model).

3.1 Introduction

The anisotropic hyperelastic constitutive model proposed by Holzapfel et al. (2000) (henceforth referred to as the HGO model) is used extensively to model collagen fibre-reinforced biological materials, even more so now that it has been implemented in several commercial and open-source Finite Element (FE) codes for the simulation of soft tissue elasticity.

The constitutive equation builds upon previously published transversely isotropic constitutive models (e.g. Weiss et al. (1996)) and reflects the structural components of a typical biological soft tissue, and hence its strain-energy density consists of two mechanically equivalent terms accounting for the anisotropic contributions of the reinforcing fibre families, in addition to a term representing the isotropic contribution of the ground matrix in which the fibres are embedded. Also, it assumes that the collagen fibres do not support compression, and hence they provide a mechanical
contribution only when in tension (this may be taken care of by pre-multiplying each anisotropic term with a Heaviside, or “switching”, function).

For the original incompressible HGO model the strain energy $\Psi$ is expressed as a function of one isochoric isotropic deformation invariant (denoted $I_1$) and two isochoric anisotropic invariants (denoted $I_4$ and $I_6$). A Lagrange multiplier is used to enforce incompressibility (Holzapfel, Gasser, and Ogden, 2000). Once again it should be stressed that the original HGO model is intended only for the simulation of incompressible materials.

A modification of the original HGO model commonly implemented in finite element codes entails the replacement of the Lagrange multiplier penalty term with an isotropic hydrostatic stress term that depends on a user specified bulk modulus. This modification allows for the relaxation of the incompressibility condition and we therefore refer to this modified formulation as the HGO-C (compressible) model for the remainder of this study.

The HGO-C model has been widely used for the finite element simulation of many anisotropic soft tissues. For example, varying degrees of compressibility have been reported for cartilage in the literature (e.g. Guilak et al. (1995); Smith et al. (2001)). It has been modelled as a compressible material using the HGO-C model (e.g. Peña et al. (2007) used a Poisson’s ratio, $\nu = 0.1$ and Pérez del Palomar and Doblaré (2006) used $\nu = 0.1$ and $\nu = 0.4$). To date, material compressibility of arterial tissue has not been firmly established. Incompressibility was assumed by the authors of the original HGO model and in subsequent studies (e.g. Kiousis et al. (2009)). However many studies model arteries as compressible or slightly compressible (e.g. Cardoso et al. (2014) $\nu = 0.33 - 0.43$ and Iannaccone et al. (2014) $\nu = 0.475$). In addition to arterial tissue the nucleus pulposus of an intervertebral disc has been modelled as a compressible anisotropic material using the HGO-C model (e.g. Maquer et al., 2014 $\nu = 0.475$). Furthermore the HGO-C
formulation has been used to simulate growth of anisotropic biological materials, where volume change is an intrinsic part of a bio-mechanical process (e.g. (Huang et al., 2012) \( \nu = 0.3 \)). However, the enforcement of perfect incompressibility may not be readily achieved in numerical models. As an example, the finite element solver Abaqus/Explicit assigns a default Poisson’s ratio of 0.475 to “incompressible” materials in order to achieve a stable solution (Abaqus.V6.11, 2001) and in this case the HGO-C model must be used (e.g. Conway et al. (2012); Famaey et al. (2012)). Despite the widespread use of the HGO-C model, its ability to correctly simulate anisotropic compressible material behaviour has not previously been established.

- The first objective of this study is to demonstrate that the HGO-C formulation does not correctly model an anisotropic compressible hyperelastic material.

Recently, Vergori et al. (2013) showed that under hydrostatic tension, a sphere consisting of a slightly compressible HGO-C material expands into a larger sphere instead of deforming into an ellipsoid. It was suggested that this effectively isotropic response is due to the isochoric anisotropic invariants \( \bar{I}_i \) being used in the switching function instead of the full invariants \( I_i, i = 4, 6 \). However, in the current paper we show that the problem emerges fundamentally because there is no dilatational contribution to the anisotropic terms of \( \Psi \). In fact, modifying only the “switching criterion” for fibre lengthening is not sufficient to fully redress the problem.

- The second objective of the study is to implement a modification of the HGO-C model so that correct anisotropic behaviour of compressible materials is achieved.

This modified anisotropic (MA) model uses the full form of the anisotropic invariants and through a range of case studies we show this leads to the correct computation of stress in contrast to the widely used HGO-C model.
The paper is structured as follows. In Section 3.2 we demonstrate and highlight the underlying cause of the insensitivity of the anisotropic component of the HGO-C model to volumetric deformation in compressible materials. We demonstrate that the modification of the model to include the full form of the anisotropic invariants corrects this deficiency. In Section 3.3 we show how the HGO-C model yields unexpected and unphysical results for pure in-plane shear and likewise in 3.4 for simple uniaxial stretching, in contrast to the modified model. We devote Section 3.5 to two Finite Element biomechanics case studies, namely pressure expansion of an artery and stent deployment in an artery, and illustrate the significant differences in computed results for the HGO-C model and the modified model. Finally, we provide some concluding remarks and discussion points in Section 3.6.

3.2 Theory: Compressible Anisotropic Hyperelastic Constitutive Models

3.2.1 HGO-C Model for Compressible Materials

The original HGO model is intended for incompressible materials. However a variation of the HGO model whereby a bulk modulus is used instead of a penalty term has been implemented in a number of FE codes. Several authors have used this formulation to model compressible anisotropic materials but using a relatively low value of bulk modulus. An important objective of this paper is to highlight that this HGO-C formulation does not correctly model compressible anisotropic material behaviour.

The kinematics of deformation are described locally in terms of the deformation gradient tensor, denoted $\mathbf{F}$, relative to some reference configuration. The right Cauchy–Green tensor is defined by $\mathbf{C} = \mathbf{F}^T \mathbf{F}$, where $^T$ indicates the transpose of a second-order tensor.
Hyperelastic constitutive models used for rubber-like materials often split the local deformation into volume-changing (volumetric) and volume-preserving (isochoric, or deviatoric) parts. Accordingly, the deformation gradient $\mathbf{F}$ is decomposed multiplicatively as follows:

\[
\mathbf{F} = \left( J^{\frac{1}{3}} \mathbf{I}_1 \right) \mathbf{F}_I,
\]

where $J$ is the determinant of $\mathbf{F}$. The term in the brackets represents the volumetric portion of the deformation gradient and $\mathbf{F}_I$ is its isochoric portion, such that $\det(\mathbf{F}_I) = 1$ at all times.

Suppose that the material consists of an isotropic matrix material within which are embedded two families of fibres characterized by two preferred directions in the reference configuration defined in terms of two unit vectors $\mathbf{a}_{0i}$, $i = 4, 6$. With $\mathbf{C}$, $J$ and $\mathbf{a}_{0i}$ are defined the invariants

\[
I_1 = \text{tr}(\mathbf{C}), \quad I_4 = \mathbf{a}_{04} \cdot (\mathbf{Ca}_{04}), \quad I_6 = \mathbf{a}_{06} \cdot (\mathbf{Ca}_{06}),
\]

\[
\bar{I}_1 = J^{-2/3}I_1, \quad \bar{I}_4 = J^{-2/3}I_4, \quad \bar{I}_6 = J^{-2/3}I_6,
\]

where $\bar{I}_i$ ($i = 1, 4, 6$) are the isochoric counterparts of $I_i$. The HGO model proposed by Holzapfel et al. (2000) for collagen reinforced soft tissues additively splits the strain energy $\Psi$ into volumetric, isochoric isotropic and isochoric anisotropic terms,
\[ \Psi(C, a_{o4}, a_{o6}) = \Psi_{\text{vol}}(J) + \Psi_{\text{iso}}(\overline{C}) + \Psi_{\text{aniso}}(\overline{C}, a_{o4}, a_{o6}), \]  

(3.4)

where \( \Psi_{\text{iso}} \) and \( \Psi_{\text{aniso}} \) are the isochoric isotropic and isochoric anisotropic free-energy contributions, respectively, and \( \overline{C} = J^{-2/3}C \) is the isochoric right Cauchy–Green deformation tensor.

In numerical implementations of the model (Abaqus V6.11, 2001; ADINA, 2005; Gasser and Holzapfel, 2002), the volumetric and isochoric isotropic terms are represented by the slightly compressible neo-Hookean hyperelastic free energy

\[ \Psi_{\text{vol}}(J) = \frac{1}{2} \kappa_0 (J - 1)^2, \quad \Psi_{\text{iso}}(\overline{C}) = \frac{1}{2} \mu_0 (\overline{I}_1 - 3), \]  

(3.5)

where \( \kappa_0 \) and \( \mu_0 \) are the bulk and shear moduli, respectively, of the soft isotropic matrix. Of course one may write Equation (3.5) in terms of the full invariants also, using the results from Equation (3.3).

The isochoric anisotropic free-energy term is prescribed as

\[ \Psi_{\text{aniso}}(\overline{C}, a_{o4}, a_{o6}) = \frac{k_1}{2k_2} \sum_{i=4,6} \{ \exp[k_2 (\overline{I}_i - 1)^2] - 1 \}, \]  

(3.6)

where \( k_1 \) and \( k_2 \) are positive material constants which can be determined from experiments.

For a general hyperelastic material with free energy \( \Psi \) the Cauchy stress is given
by

\[ \sigma = \frac{1}{J} F \frac{\partial \Psi}{\partial F} \]  

(3.7)

For the Cauchy stress derived from \( \Psi \) above, we have the decomposition \( \sigma = \sigma_{\text{vol}} + \sigma_{\text{iso}} + \sigma_{\text{aniso}} \), where

\[ \sigma_{\text{vol}} = \kappa_0 (J - 1) I, \quad \sigma_{\text{iso}} = \mu_0 J^{-1} \left( \overline{b} - \frac{1}{3} I_1 I \right), \]  

(3.8)

with \( \overline{b} = \overline{F} F^T \), and

\[ \sigma_{\text{aniso}} = 2k_1 J^{-1} \sum_{i=4,6} (\overline{I}_i - 1) \exp[k_2 (\overline{I}_i - 1)^2] (\overline{a}_i \otimes \overline{a}_i - \frac{1}{3} I_1 I), \]  

(3.9)

where \( \overline{a}_i = \overline{F} a_{0i} \). This slightly compressible implementation is referred to as the HGO-C model henceforth.

The original incompressible HGO model by Holzapfel et al. (2000) specified that for arteries the constitutive formulation should be implemented for incompressible materials. In that limit, \( \kappa_0 \to \infty, \quad (J - 1) \to 0 \) while the product of these two quantities becomes an indeterminate Lagrange multiplier, \( p \), and the volumetric stress assumes the form, \( \sigma_{\text{vol}} = -p I \). Indeed the original incompressible HGO model can equally be expressed in terms of the full invariants \( I_4 \) and \( I_6 \) (with \( J \to 1 \)) (e.g., Holzapfel et al. (2004)).

However, in the case of the HGO-C implementation, if \( \kappa_0 \) is not fixed numerically at a large enough value, then slight compressibility is introduced into the model. The key point of this paper is that the isochoric anisotropic term \( \Psi_{\text{aniso}} \) defined in Equation (3.6) does not provide a full representation of the anisotropic contributions
to the stress tensor for slightly compressible materials. In Section 3.2.4 we introduce a simple modification of the anisotropic term to account for material compressibility.

### 3.2.2 Pure dilatational deformation

First we consider the case of the HGO-C material subjected to a pure dilatation with stretch $\lambda = J^{1/3}$, so that

$$F = \lambda I, \quad C = \lambda^2 I, \quad J = \lambda^3.$$  \hspace{1cm} (3.10)

We expect that an anisotropic material requires an anisotropic stress state to maintain the pure dilatation. However, calculation of the invariants $I_i$ and $\bar{I}_i$ yields

$$I_i = a_{0i} \cdot (Ca_{0k}) = \lambda^2, \quad \bar{I}_i = J^{-2/3}I_i = 1, \quad i = 4, 6,$$  \hspace{1cm} (3.11)

so that while $I_i$ is indeed the square of the fibre stretch and changes with the magnitude of the dilatation, its isochoric counterpart $\bar{I}_i$ is always unity. Referring to Equation (3.9), it is clear that the entire anisotropic contribution to the stress Equation (3.7) disappears (i.e. $\sigma_{\text{aniso}} \equiv 0$), and the remaining active terms are the isotropic ones. Thus, under pure dilatation, the HGO-C model computes an entirely isotropic state of stress.
3.2.3 Applied hydrostatic stress

Now we investigate the reverse question: what is the response of the HGO-C material to a hydrostatic stress,

$$\sigma = \sigma I,$$

where $\sigma > 0$ under tension and $\sigma < 0$ under pressure? In an anisotropic material, we expect the eigenvalues of $C$, the squared principal stretches, $\lambda_1^2, \lambda_2^2, \lambda_3^2$ say, to be distinct. Hence, if the material is slightly compressible, then a sphere should deform into an ellipsoid (Vergori et al., 2013) and a cube should deform into a hexahedron with non-parallel faces (Annaidh et al., 2013).

However, in the HGO-C model the $\Psi_{\text{aniso}}$ contribution is switched on only when $I_i$ (not $I_1$) is greater than unity. Vergori et al. (2013) showed that in fact $I_i$ is always less than or equal to one in compression and in expansion under hydrostatic stress, so that the HGO-C response is isotropic, contrary to physical expectations. Then we may ask if removal of the switching function circumvents this problem so that anisotropic response is obtained.

With the fibres taken to be mechanically equivalent and aligned with $a_{04} = (\cos \Theta, \sin \Theta, 0)$ and $a_{06} = (\cos \Theta, -\sin \Theta, 0)$ in the reference configuration, we have, by symmetry, $I_6 = I_4$ and $\bar{T}_6 = \bar{T}_4$ and $\bar{\Psi}_6 = \bar{\Psi}_4$, where the subscripts 4 and 6 on $\bar{\Psi}$ signify partial differentiation with respect to $\bar{T}_4$ and $\bar{T}_6$, respectively. Similarly, in the following the subscript 1 indicates differentiation with respect to $\bar{T}_1$. For this special case, Vergori et al. (2013) showed that the stretches arising from the
application of a hydrostatic stress are

\[
\lambda_1 = J^{1/3} \left[ \frac{\Psi_1(\Psi_1 + 2\Psi_4 \sin^2 \Theta)}{(\Psi_1 + 2\Psi_4 \cos^2 \Theta)^2} \right]^{\frac{1}{6}},
\]

\[
\lambda_2 = J^{1/3} \left[ \frac{\Psi_1(\Psi_1 + 2\Psi_4 \cos^2 \Theta)}{(\Psi_1 + 2\Psi_4 \sin^2 \Theta)^2} \right]^{\frac{1}{6}},
\]

\[
\lambda_3 = J^{1/3} \left[ \frac{\Psi_1^2 + 2\Psi_1 \Psi_4 + \Psi_4^2 \sin^2 2\Theta}{\Psi_1^2} \right]^{\frac{1}{6}}. \tag{3.13}
\]

Explicitly,

\[
\Psi_1 = \frac{\partial \Psi}{\partial I_1} = \frac{1}{2} \mu_0, \quad \Psi_4 = \frac{\partial \Psi}{\partial I_4} = k_1(I_4 - 1) \exp[k_2 (I_4 - 1)^2]. \tag{3.14}
\]

Looking at Equation (3.13), we see that there is a solution to the hydrostatic stress problem where the stretches are unequal, so that a sphere deforms into an ellipsoid. However, there is also another solution: that for which \( I_4 \equiv 1 \), in which case, \( \Psi_4 \equiv 0 \) by the above equation, and then \( \lambda_1 = \lambda_2 = \lambda_3 = J^{1/3} \) by Equation (3.13). Thus, a sphere then deforms into another sphere.

Of those (at least) two possible paths, FE solvers converge upon the isotropic solution. One possible explanation for this may be that the initial computational steps calculate strains in the small-strain regime. In that regime, Vergori et al. (2013) showed that all materials with a decoupled volumetric/isochoric free-energy behave in an isotropic manner when subject to a hydrostatic stress. Hence the first computational step brings the deformation on the isotropic path, and then subsequently. In Section 3.2.2 and Section 3.2.3 we have thus demonstrated that the use of an isochoric form of the anisotropic strain energy \( \Psi_{aniso} \) from the HGO model in the HGO-C model cannot yield a correct response to pure dilatation.
or applied hydrostatic stress.

3.2.4 Modified Anisotropic Model for Compressible Materials

In order to achieve correct anisotropic behaviour for compressible materials we introduce a modification to the anisotropic term of the HGO model, whereby the anisotropic strain energy is a function of the ‘total’ right Cauchy–Green deformation tensor $C$, rather than its isochoric part $\overline{C}$, so that

$$
\Psi (J, C, a_{04}, a_{06}) = \Psi_{\text{vol}} (J) + \Psi_{\text{iso}} (J, C) + \Psi_{\text{aniso}} (C, a_{04}, a_{06}),
$$

(3.15)

where the expressions for strain energy density terms $\Psi_{\text{vol}}$ and $\Psi_{\text{iso}}$ are the same as $\Psi_{\text{vol}}$ and $\Psi_{\text{iso}}$ in Equation (3.5), and

$$
\Psi_{\text{aniso}} (C, a_{04}, a_{06}) = \frac{k_1}{2k_2} \sum_{i=4,6} \{ \exp[k_2 (I_i - 1)^2] - 1 \}.
$$

(3.16)

This modification to the HGO-C model is referred to as the modified anisotropic (MA) model hereafter. Combining Equation (3.5), Equation (3.15) and Equation (3.16), the Cauchy stress for the MA model is determined using Equation (3.7) and the decomposition $\sigma = \sigma_{\text{vol}} + \sigma_{\text{iso}} + \sigma_{\text{aniso}}$ resulting in the expression:

$$
\sigma = \kappa_0 (J - 1)I + \mu_0 J^{-5/3} (b - \frac{1}{3} I_1 I) + 2k_1 \sum_{i=4,6} (I_i - 1) \exp[k_2 (I_i - 1)^2] a_i \otimes a_i.
$$

(3.17)

where $a_i = \mathbf{F}a_{0i}, i = 4, 6$. Now it is easy to check that in the cases of a pure dilatation and of a hydrostatic stress, the MA model behaves in an anisotropic
manner, because the term $I_i - 1 \neq 0$ and hence $\Psi_{\text{aniso}} \neq 0$ and $\sigma_{\text{aniso}} \neq 0$. This resolves the issues identified above for the HGO-C model.

We have developed a user-defined material model (UMAT) Fortran subroutine to implement the MA formulation for the Abaqus/Standard FE software. The FE implicit solver requires that both the Cauchy stress and the consistent tangent matrix (material Jacobian) are returned by the subroutine. Appendix A gives the details of the consistent tangent matrix.

We have used the above subroutine to repeat the simulations of expansion of a sphere under hydrostatic tension of Vergori et al. (2013), this time using the MA formulation. Again two families of fibres are assumed, lying in the $(1, 2)$ plane and symmetric about the $I$-axis (the sphere and axes are shown in Figure 3.1A). The displacements of points on the surface of the sphere at the ends of three mutually orthogonal radii with increasing applied hydrostatic tension are shown in Figure 3.1B. Clearly the sphere deforms into an ellipsoid with a major axis oriented in the 3-direction and a minor axis oriented in the 1-direction, confirming the simulation of orthotropic material behaviour. The distribution of stress triaxiality in the deformed ellipsoid, measured by $\sigma_{\text{hyd}}/q$, is shown in Figure 3.1C, where $\sigma_{\text{hyd}} \equiv \text{tr}(\sigma)/3$ is the hydrostatic stress and $q \equiv \sqrt{3/2} \sigma' : \sigma'$ is the von Mises equivalent stress, $\sigma'$ being the deviatoric Cauchy stress tensor. Clearly an inhomogeneous stress state is computed in the deformed body.

The results shown in Figure 3.1 contrast sharply with the equivalent simulations using the HGO-C model (Vergori et al., 2013) superimposed in Figure 3.1B for comparison. In that case a similar fibre-reinforced sphere is shown to deform into a larger sphere with a homogeneous stress distribution, indicative of isotropic material behaviour.
Figure 3.1:  A) Schematic of an undeformed sphere highlighting three radii on orthogonal axes, 1-2-3, centred at the sphere origin. Two families of fibres are contained in the (1, 2) plane and symmetric about the 1-axis. B) Computed (deformed/undeformed) ratios \( r/r_0 \) of the orthogonal radii for both MA and HGO-C models versus the ratio \( \sigma_{\text{hyd}}/\sigma_{\text{max}}^{\text{hyd}} \). Note that the deformation computed for the HGO-C model incorrectly remains spherical. C) Deformed ellipsoidal shape computed for the MA model; contours illustrate the inhomogeneous distribution of stress triaxiality \( (\sigma_{\text{hyd}}/q) \) throughout the deformed body.

3.3 Analysis of Pure Shear

A pure dilatation and a hydrostatic stress each represent a highly idealized situation, unlikely to occur by themselves in soft tissue in vivo. This section highlights the unphysical behaviour can also emerge for common modes of deformation if the anisotropic terms are based exclusively on the isochoric invariants. Considering once again the general case of a compressible anisotropic material, we analyse the response of the HGO-C and MA models to pure in-plane shear. Regarding the out-of-plane boundary conditions, we first consider the case of plane strain (Section 3.3.1). Even though this deformation is entirely isochoric the HGO-C model yields incorrect results. We then consider the case of plane stress (Section 3.3.2), and again demonstrate that the HGO-C model yields incorrect results. By contrast, we show that the MA model computes a correct stress state for all levels of compressibility and specified deformations. In the following calculations we assume a shear mod-
ulus, $\mu_0 = 0.05 \text{MPa}$ and anisotropic material constants $k_1 = 1 \text{MPa}$ and $k_2 = 100$ (Vergori et al., 2013).

### 3.3.1 Plane strain pure shear

With restriction to the $(1, 2)$ plane we now consider the plane strain deformation known as *pure shear*, maintained by the application of a suitable Cauchy stress. In particular, we take the deformation gradient for this deformation to have components

$$
F = \begin{bmatrix}
\sqrt{F_{12}^2 + 1} & F_{12} & 0 \\
F_{12} & \sqrt{F_{12}^2 + 1} & 0 \\
0 & 0 & 1
\end{bmatrix},
$$

(3.18)

where $F_{12}$ is a measure of the strain magnitude. Figure 3.2A depicts the deformation of the $(1, 2)$ square cross section of a unit cube, which deforms into a parallelogram symmetric about a diagonal of the square. The deformation corresponds to a stretch $\lambda = \sqrt{F_{12}^2 + 1} + F_{12}$ along the leading diagonal with a transverse stretch $\lambda^{-1} = \sqrt{F_{12}^2 + 1} - F_{12}$. We can think of the deformation arising from displacement components applied to the vertices of the square, as indicated in Figure 3.2A. Two families of fibres, with reference unit vectors $a_{04}$ and $a_{06}$ are assumed to lie in the $(1, 2)$ plane, as illustrated in Figure 3.2A, oriented with angles $\pm \theta$ to the 1 axis. We perform some calculations for a range of fibre orientations for each of the HGO-C and MA models.

First we note that although, for this specific case, the free energies of the HGO-C and the MA models coincide (because $J = 1$ and hence $I_4 = T_4$), the corresponding stress tensors are very different. This is due to the “deviatoric” form of the anisotropic stress contribution that emerges for the HGO-C model, as in the final
Figure 3.2: A) Schematic illustrating the kinematics of the pure shear deformation of the \((1,2)\) section of a unit cube. Note the rotated coordinate system \((1',2')\), orientated at \(45^\circ\) to the \((1,2)\) axes, used to specify the vertex displacement components \(u_{1'}\) and \(u_{2'}\). Note also the vectors \(a_0\), \(i = 4, 6\), indicating the directions of the two families of fibres, with angle \(\theta\). Results are displayed for a range of fibre orientations with \(\theta\) from \(\pm 45^\circ\) to \(\pm 90^\circ\) with respect to the \((1,2)\) coordinate system. B) Computed stress ratio \(\sigma_{33}/\sigma_{12}\) versus \(F_{12}\) for the HGO-C model, illustrating significant negative (compressive) stresses in the out-of-plane direction. C) Computed stress ratio versus \(F_{12}\) for the MA model, illustrating very small negative (compressive) stresses in the out-of-plane direction (an order of magnitude lower than for the HGO-C model).

The term of Equation (3.9), compared with the final term of Equation (3.17). It gives rise to a significant negative (compressive) out-of-plane stress component \(\sigma_{33}\) which is comparable in magnitude to \(\sigma_{12}\), as shown in Figure 3.2B. Such a negative stress is anomalous in the sense that for large \(\kappa_0\) the result for the incompressible limit should be recovered, but it is not. Indeed, if we start with the incompressible model we obtain \(\sigma_{33} = \mu_0 - p\), which is independent of \(\sigma_{12}\). However, as Equation (3.18) represents a kinematically prescribed isochoric deformation, the volumetric stress in the HGO-C model goes to zero and does not act as the required Lagrange multiplier.

By contrast, the out-of-plane compressive normal stress component \(\sigma_{33}\) computed for the MA model is at least an order of magnitude lower than the in-plane shear stress component \(\sigma_{12}\) (Figure 3.2C), and is close to zero for most fibre orientations.
This is consistent with the incompressible case because, since $p$ is arbitrary it may be chosen to be $\mu_0$ so that $\sigma_{33} = 0$. This is what might be expected physically, given that the fibres and the deformations are confined to the (1, 2) plane.

Because of the deviatoric component of the stress tensor emerging from the HGO-C model, the trace of the Cauchy stress is always zero when $J = 1$ as equations Equation (3.8) and Equation (3.9) will confirm. By contrast, the trace of the Cauchy stress is not zero for the MA model. Hence the in-plane stress components are significantly different from those for the HGO-C model, as shown in Figures 3.3A and 3.3B, respectively, for the case of a single fibre family with $\theta = 30^\circ$.

### 3.3.2 Plane stress pure shear

The kinematically prescribed isochoric deformation in Section 3.3.1 is volume conserving and makes the $\Psi_{\text{vol}}$ terms equal to zero. We modify the out-of-plane boundary condition to enforce a plane stress ($\sigma_{33} = 0$) simulation. This allows a compressible material to deform of out-of-plane.
A plane stress pure shear deformation is given as

\[
\mathbf{F} = \begin{bmatrix}
\sqrt{F_{12}^2 + 1} & F_{12} & 0 \\
F_{12} & \sqrt{F_{12}^2 + 1} & 0 \\
0 & 0 & F_{33}
\end{bmatrix},
\tag{3.19}
\]

where the out of plane stretch component \(F_{33}\) in general is not equal to 1, so that the deformation is not in general isochoric. If the bulk modulus \(\kappa_0\) is very large compared with the initial shear modulus \(\mu_0\), then it acts as a Lagrange multiplier to enforce incompressibility, such that \(F_{33} = 1\) (at least approximately). If the magnitude of the bulk modulus is reduced, then the material becomes slightly compressible and \(F_{33} \neq 1\). Here we investigate the sensitivity of the stress computed for the HGO-C and MA models to the magnitude of the bulk modulus \(\kappa_0\).

First, we consider the almost incompressible case where the ratio of bulk to shear modulus is \(\kappa_0/\mu_0 = 2 \times 10^6\) for the isotropic neo-Hookean component of the model, equivalent to an effective Poisson ratio of \(\nu = 0.49999975\). This effective Poisson’s ratio is calculated using Equation (3.20).

\[
\nu_{\text{eff}} = \frac{3\kappa_0/\mu_0 - 2}{6\kappa_0/\mu_0 + 2}.
\tag{3.20}
\]

The stress components are shown in Figure 3.4A. An important point to note is that in this case the deformation is effectively isochoric, because we find \(J = F_{33} = 1.00006\), and yet the HGO-C model predicts an entirely different stress state from that for the kinematically constrained isochoric deformation of the previous section shown in Figure 3.3B. This is because the volumetric term of the free energy now contributes to the trace of the stress tensor, and therefore the high magnitude of bulk modulus effectively acts as a Lagrange multiplier to enforce incompressibility.
Figure 3.4: Dimensionless plots of the normal and in-plane shear Cauchy stress components $\sigma_{ij}/k_1$ versus $F_{12}$ for the case of a single family of fibres orientated at $\theta = 30^\circ$. A) Computed stresses for both the HGO-C and MA models with a large bulk modulus $\kappa_0/\mu_0 = 2 \times 10^6$ (equivalent to a Poisson ratio of 0.49999975). Note that the plots for both models are perfectly overlaid upon each other. B) Computed stresses for the HGO-C model with $\kappa_0/\mu_0 = 50$ (equivalent to a Poisson ratio of 0.490). Note that the stresses computed for the HGO-C model are an order of magnitude lower in the slightly compressible small bulk modulus case than in the almost incompressible large bulk modulus case.

Indeed for these conditions the HGO-C and MA models behave identically to the original HGO model. However, unlike the HGO-C model, the MA model computes identical stress components for both the kinematically constrained isochoric deformation Equation (3.18) and for the Lagrange multiplier enforced volume preserving deformation Equation (3.19).

If the incompressibility constraint is slightly relaxed, so that $\kappa_0/\mu_0 = 50$ ($\nu = 0.490$) the HGO-C model computes a very different stress state, as shown in Figure 3.4B, with stress components being reduced by an order of magnitude. Thus the HGO-C model is very sensitive to changes in the bulk modulus and, consequently, incompressibility must be enforced by choosing a very large magnitude for the bulk modulus in order to avoid the computation of erroneous stress states.
By contrast, the MA model computes identical stress states for $\frac{\kappa_0}{\mu_0} = 2 \times 10^6$ and $\frac{\kappa_0}{\mu_0} = 50$ (Figure 3.4A in both cases). This response highlights the robustness of the MA model, which computes correct results for all levels of material compressibility (including the incompressible limit).

### 3.4 Uniaxial stretch

We now consider a confined uniaxial stretch, as illustrated in Figure 3.5A, where a stretch is imposed in the 2-direction ($\lambda_2 = \lambda > 1$) and no lateral deformation is permitted to occur in the 1- and 3-directions ($\lambda_1 = \lambda_3 = 1$). Such a simple deformation may have biomechanical relevance as, for example, in a blood vessel undergoing large circumferential strain, but little or no axial or radial strain.

**Figure 3.5:**  
A) Schematic of confined uniaxial stretch ($\lambda_2 = \lambda > 1, \lambda_1 = \lambda_3 = 1$), showing the fibre family reference directional vector $a_0$ in the (1, 2) plane. The ratio of the Cauchy stress components $\sigma_{11}/\sigma_{22}$ is computed based on a model with a single fibre family and plotted as a function of $\lambda$. Results are displayed for a range of fibre orientations $\theta$ from $0^\circ$ to $90^\circ$.  
B) Computed results for the HGO-C model, illustrating negative (compressive) lateral stresses.  
C) Computed results for the MA model, all lateral stresses being positive (tensile).

We derive analytically the stress components for the HGO-C and MA models using the formulas of Section 3.2. We assume there is a single family of parallel fibres.
aligned with the reference unit vector $a_0$ in the $(1, 2)$ plane and with orientation $\theta$ relative to the 1-axis ranging from $0^\circ$ to $90^\circ$. We take $\mu_0 = 0.05 \text{ MPa}$, $\kappa_0 = 1 \text{ MPa}$ for the slightly compressible neo-Hookean isotropic matrix, and material constants $k_1 = 1 \text{ MPa}$ and $k_2 = 100$ for the fibre parameters.

The ratio of the lateral to axial Cauchy stress components, $\sigma_{11}/\sigma_{22}$, is plotted as a function of applied stretch $\lambda$ for the HGO-C model (Figure 3.5B) and the MA model (Figure 3.5C). Results for the HGO-C model exhibit negative (compressive) stresses in the lateral direction for certain fibre orientations. This auxetic effect suggests that the material would expand in the lateral direction in the absence of the lateral constraint and is contrary to expectations, particularly for fibre orientations closer to the axial direction. In fact, here the computed lateral compressive force is most pronounced when the fibre is aligned in the direction of stretch ($\theta = 90^\circ$), where a transversely isotropic response, with exclusively tensile lateral stresses, should be expected. For all fibres orientated within about $45^\circ$ of the direction of stretch, the lateral stress changes from tensile to compressive as the applied stretch increases. By contrast to the HGO-C model, the MA model yields exclusively tensile lateral stresses for all fibre orientations (Figure 3.5C).

### 3.5 Finite Element analysis of realistic arterial deformation

Following from the idealized, analytical deformations considered above, we now highlight the practical significance of the errors computed by using the HGO-C model for slightly compressible tissue. We consider, in turn, two Finite Element case studies using Abaqus.V6.11 (2001) to implement the HGO-C and MA models with user-defined material subroutines (see Appendix A).
3.5.1 Pressure expansion of an artery

First we simulate the deformation of an artery under a lumen pressure ($LP$). A schematic of a quarter artery is shown in Figure 3.6A. The vessel has an internal radius $r_1$ of 0.6 mm and an external radius $r_e$ of 0.9 mm. The length of the artery in the $z$-direction is 0.3 mm with both ends constrained in the $z$-direction.

We model the wall as a homogeneous material with two families of fibres lying locally in the ($\theta, z$) plane, where ($r, \theta, z$) are cylindrical polar coordinates. The fibre families are symmetric with respect to the circumferential direction and oriented at $\pm 50^\circ$ measured from the circumferential direction. For the fibres, the material constants are $k_1 = 1$ MPa and $k_2 = 2$, and for the neo-Hookean matrix, they are $\mu_0 = 0.03$ MPa, $\kappa_0 = 1$ MPa, resulting in a slightly incompressible material (corresponding to a Poisson ratio of 0.485). A mesh sensitivity study confirms a converged solution for a model using a total of 1,044 eight-noded full-integration hexahedral elements.

The (dimensionless) changes in the internal and external radii $\Delta r/r_0$ as functions of increasing dimensionless lumen pressure $LP/LP_{max}$ are plotted in Figure 3.6B. They reveal that the HGO-C model predicts a far more compliant artery than the MA model.

Notable differences in the arterial wall stress state arise between the HGO-C and MA models. Figures 3.6C, D and E present the von Mises stress, pressure stress and triaxiality, respectively, in the arterial wall. The magnitude and gradient through the wall thickness of both the von Mises stress and pressure stress differ significantly between the HGO-C and MA models. This contrast is further highlighted by the differing distributions of triaxiality for both models, confirming a fundamental difference in the multi-axial stress state computed for the two models.
Figure 3.6:  

**A)** Schematic illustrating the geometry, lines of symmetry and boundary conditions for modelling the inflation of an artery under a lumen pressure $LP$.  

**B)** Prediction of the internal ($r_i$) and external ($r_e$) radial strain $\Delta r/r_0 = (r - r_0)/r_0$ in the artery under a normalized lumen pressure $LP/LP_{\text{max}}$ for the HGO-C and MA models. Panels **C)**, **D)** and **E)** are contour plots illustrating the von Mises ($q$), pressure ($-\sigma_{\text{hyd}}$) and triaxiality ($\sigma_{\text{hyd}}/q$) stresses, respectively, in the artery wall for the HGO-C and MA models.
Figure 3.7: Plot of the dimensionless radial force \( \frac{(F - F_0)}{F_0} \) required to deploy a stent in an artery with increasing stent radial expansion. Radial force is normalized by the radial force at the point immediately before contact with the artery \( (F_0) \). The radial expansion is normalized using the initial undeformed internal radius \( (r_i) \) and the final fully deployed internal radius \( (r_f) \). Note that the HGO-C model predicts a more compliant artery than the MA model.
3.5.2 Stent deployment in an artery

The final case study examines the deployment of a stainless steel stent in a straight artery. Nowadays most medical device regulatory bodies insist on computational analysis of stents (FDA, 2010) as part of their approval process. Here we demonstrate that the correct implementation of the constitutive model for a slightly compressible arterial wall is critical for the computational assessment of stent performance.

We use a generic closed-cell stent geometry (Conway et al., 2012) with an undeformed radius of 0.575 mm. It is made of biomedical grade stainless steel alloy 316L with Young’s modulus of 200 GPa and Poisson’s ratio 0.3 in the elastic domain. We model plasticity using isotropic hardening $J_2$-plasticity with a yield stress of 264 MPa and ultimate tensile strength of 584 MPa at a plastic log strain of 0.274 McGarry et al. (2007). We mesh the stent geometry with 22,104 reduced integration hexahedral elements. We model a balloon using membrane elements, with frictionless contact between the membrane elements and the internal surface of the stent. Finally, we simulate the balloon deployment by imposing radial displacement boundary conditions on the membrane elements.

For the artery, we take a single layer with two families of fibres symmetrically disposed in the $(\theta, z)$ plane. The fibres are oriented at $\pm 50^\circ$ to the circumferential direction and material constants and vessel dimensions are the same as those used in Section 3.5.1. Here the FE mesh consists of 78,100 full integration hexahedral elements; a high mesh density is required due to the complex contact between the stent and the artery during deployment.

“Radial stiffness”, the net radial force required to open a stent, is a commonly cited measure of stent performance (FDA, 2010). Figure 3.7 presents plots of the predicted net radial force as a function of radial expansion for the HGO-C and MA models. The predicted radial force required to expand the stent to the final diameter is significantly lower for the HGO-C model than for the MA model. This
Figure 3.8: Contour plots illustrating differences in the stresses computed for the HGO-C and MA models after stent deployment. **A)** von Mises stress $q$, **B)** pressure stress $-\sigma_{hyd}$, **C)** triaxiality, **D)** ratio of axial stress to the circumferential stress $\sigma_{zz}/\sigma_{\theta\theta}$. 
result correlates with the previous finding in Section 3.5.1 that the HGO-C model underestimates the arterial compliance, with significant implications for design and assessment of stents.

Figure 3.8 illustrates the notable differences that appear in the artery stress state between the HGO-C and MA models. Again, higher values of von Mises stress (Figure 3.8A) and pressure stress (Figure 3.8B) are computed for the MA model. Both the triaxiality (Figure 3.8C) and the ratio of axial to circumferential stress (the stress ratio in the plane of the fibres) (Figure 3.8D) confirm that the nature of the computed multi-axial stress state is significantly different between the MA and HGO-C models.

A detailed examination of the stress state through the thickness (radial direction) of the artery wall is presented in Figure 3.9. A comparison between HGO-C and MA simulations in terms of the ratios of the Cauchy stress components emphasizes further the fundamentally different stresses throughout the entire artery wall thickness. It is not merely that the MA model calculates a different magnitude of stress, rather the multi-axiality of the stress state has been altered.

### 3.6 Concluding remarks

The original HGO model ((Holzapfel et al., 2000)) is intended for modelling of incompressible anisotropic materials. A compressible form (HGO-C model) is widely used whereby the anisotropic part of \( \Psi \) is expressed in terms of isochoric invariants. Here we demonstrate that this formulation does not correctly model compressible anisotropic material behaviour. The anisotropic component of the model is insensitive to volumetric deformation due to the use of isochoric anisotropic invariants. This explains the anomolous finite element simulations reported in Vergori et al. (2013), whereby a slightly compressible HGO-C sphere was observed to deform into
Figure 3.9: Stress measures computed through the arterial wall from the internal \((r_i)\) to external radius \((r_e)\) at full deployment of the stent for the HGO-C and MA models. A) Triaxiality ratio \(\sigma_{\text{hyd}}/q\) of the pressure stress to von Mises stress. B) Ratio \(\sigma_{zz}/\sigma_{\theta\theta}\) of the axial to circumferential stress. C) Ratio \(\sigma_{rr}/\sigma_{zz}\) of the radial to axial stress. D) Ratio \(\sigma_{rr}/\sigma_{\theta\theta}\) of the radial to circumferential stress.
a larger sphere under tensile hydrostatic loading instead of the ellipsoid which would be expected for an anisotropic material. In order to achieve correct anisotropic compressible hyperelastic material behaviour we present and implement a modified (MA) model whereby the anisotropic part of the strain energy density is a function of the total form of the anisotropic invariants, so that a volumetric anisotropic contribution is represented. This modified model correctly predicts that a sphere will deform into an ellipsoid under tensile hydrostatic loading.

In the case of (plane strain) pure shear, a kinematically enforced isochoric deformation, we have shown that a correct stress state is computed for the MA model, whereas the HGO-C model yields incorrect results. Correct results are obtained for the HGO-C model only when incompressibility is effectively enforced via the use of a large bulk modulus, which acts as a Lagrange multiplier in the volumetric contribution to the isotropic terms (in this case HGO-C model is effectively the same as the original incompressible HGO model). In the case of a nearly incompressible material (with Poisson’s ratio = 0.490, for example) we have shown that the in-plane stress components computed by the HGO-C model are reduced by an order of magnitude. Bulk modulus sensitivity has been pointed out for isotropic models by Gent et al. (2007) and Destrade et al. (2012), and for the HGO-C model by Annaidh et al. (2013). Here, we have demonstrated that a ratio of bulk to shear modulus of $\kappa_0/\mu_0 = 2 \times 10^6$ (equivalent to a Poisson’s ratio of 0.49999975) is required to compute correct results for the HGO-C model. By contrast, the MA model is highly robust with correct results being computed for all levels of material compressibility during kinematically prescribed isochoric deformations.

From the view-point of general finite element implementation, red the requirement of perfect incompressibility (as in the case of a HGO material) can introduce numerical problems requiring the use of selective reduced integration and mixed finite elements to avoid mesh locking and hybrid elements to avoid ill-conditioned
stiffness matrices. Furthermore, due to the complex contact conditions in the simulation of balloon angioplasty (both between the balloon and the stent, and between the stent and the artery), explicit Finite Element solution schemes are generally required. However, Abaqus/Explicit for example has no mechanism for imposing an incompressibility constraint and assumes by default that $\kappa_0/\mu_0 = 20$ ($\nu = 0.475$). A value of $\kappa_0/\mu_0 > 100$ ($\nu = 0.495$) is found to introduce high frequency noise into the explicit solution. We have demonstrated that the HGO-C model should never be used for compressible or slightly compressible materials. Instead, due to its robustness, we recommend that the MA model is used in FE implementations because (i) it accurately models compressible anisotropic materials, and (ii) if material incompressibility is desired but can only be approximated numerically (e.g., Abaqus/Explicit) the MA model will still compute a correct stress state.

A paper by (Sansour, 2008) outlined the potential problems associated with splitting the free energy for anisotropic hyperelasticity into volumetric and isochoric contributions; see also Federico (2010) for a related discussion. A study of the HGO-C model by Helfenstein et al. (2010) considered the specific case of uniaxial stress with one family of fibres aligned in the loading, and suggested that the use of the ‘total’ anisotropic invariant $I_1$ is appropriate. The current paper demonstrates the importance of a volumetric anisotropic contribution for compressible materials, highlighting the extensive range of non-physical behaviour that may emerge in the simulation of nearly incompressible materials if the HGO-C model is used instead of the MA model. Examples including the Finite Element analysis of artery inflation due to increasing lumen pressure and stent deployment. Assuming nearly incompressible behaviour ($\nu = 0.485$) the HGO-C model is found to significantly underpredict artery compliance, with important implications for simulation and the design of stents (FDA, 2010). We have shown that the multiaxial stress state in an artery wall is significantly different for the HGO-C and MA models. Arterial wall
stress is thought to play an important role in in-stent restenosis (neo-intimal hyperplasia) (Thury et al., 2002; Wentzel et al., 2003). Therefore, a predictive model for the assessment of the restenosis risk of a stent design must include an appropriate multi-axial implementation of the artery constitutive law.

### 3.7 Appendices

To write a UMAT, we provide the Consistent Tangent Matrix (CTM) of the chosen model. When expressed in terms of Cauchy stress the CTM given in Abaqus.V6.11 (2001) may be written as

\[
c_{ijkl} = \sigma_{ij} \delta_{kl} + \frac{1}{2} \left( \frac{\partial \sigma_{ij}}{\partial F_{k\alpha}} F_{l\alpha} + \frac{\partial \sigma_{ij}}{\partial F_{l\alpha}} F_{k\alpha} \right),
\]

(3.21)

which has both the \(i \leftrightarrow j\) and \(k \leftrightarrow l\) minor symmetries.

The CTM may estimated using either numerical techniques or an analytical solution. Here we first describe a numerical technique for estimation of the CTM. We then present the analytical solution for the MA and HGO-C CTM.

**Appendix 3A Numerical Approximation of the CTM**

The CTM may be approximated numerically (Sun et al. (2008)), and a short overview is presented here. This numerical approximation is based on a linearised incremental form of the Jaumann rate of the Kirchhoff stress:

\[
\Delta \tau - \Delta W \tau - \tau \Delta W^T = c : \Delta D,
\]

(3.22)

where \(\tau\) is the Kirchhoff stress, \(\Delta \tau\) is the Kirchhoff stress rate, \(\Delta D\) the rate-of-deformation tensor and \(\Delta W\) the spin tensor are the symmetric and anti-symmetric
parts of the spatial velocity gradient $\Delta L$ (where $\Delta L = \Delta FF^{-1}$), and \( c \) is the CTM.

To obtain an approximation for each of components of the CTM, a small perturbation is applied to Equation (3.22) through $\Delta D$. This is achieved by perturbing the deformation gradient six times, once for each of the independent components of $\Delta D$, using

$$\Delta F^{(ij)} = \frac{\epsilon}{2}(e_i \otimes e_j F + e_j \otimes e_i F),$$

where $\epsilon$ is a perturbation parameter, $e_i$ is the basis vector in the spatial description, $(ij)$ denotes the independent component being perturbed.

The ‘total’ perturbed deformation gradient is given by $\hat{F}^{(ij)} = \Delta F^{(ij)} + F$. The Kirchhoff stress is then calculated using this perturbed deformation gradient $(\tau(\hat{F}^{(ij)}))$. The CTM is approximated using

$$c^{(ij)} \approx \frac{1}{J\epsilon}(\tau(\hat{F}^{(ij)}) - \tau(F)),$$

where $J$ is the determinant of the deformation gradient. Each perturbation of Equation (3.24) will produce six independent components. This is performed six times for each independent $(ij)$, giving the required $6 \times 6$ CTM matrix.

Appendix 3B Analytical solutions for the MA and HGO-C CTM

Here we present an analytical solution for the CTM for the MA and HGO models. For convenience we give the volumetric, isotropic and anisotropic contributions separately.
For the MA model the stress is given by equations Equation (3.8) and Equation (3.17). We can calculate \( c_{ijkl} \) from

\[
(\sigma_{\text{vol}})_{ij}\delta_{kl} + \frac{\partial(\sigma_{\text{vol}})_{ij}}{\partial F_{\kappa\alpha}} F_{\kappa\alpha} = \kappa_0 (2J - 1) \delta_{ij} \delta_{kl},
\]

(3.25)

\[
(\sigma_{\text{iso}})_{ij}\delta_{kl} + \frac{\partial(\sigma_{\text{iso}})_{ij}}{\partial F_{\kappa\alpha}} F_{\kappa\alpha} = \mu_0 J^{-1} (B_{jl}\delta_{ik} + B_{il}\delta_{jk} - \frac{2}{3} B_{kl}\delta_{ij} + \frac{2}{3} \bar{T}_{1}\delta_{ij} \delta_{kl}),
\]

(3.26)

\[
(\sigma_{\text{aniso}})_{ij}\delta_{kl} + \frac{\partial(\sigma_{\text{aniso}})_{ij}}{\partial F_{\kappa\alpha}} F_{\kappa\alpha} = 2k_1 J^{-1} \sum_{n=4,6} (I_n - 1) \exp[k_2 (I_n - 1)^2] (a_{nj} a_{nl}\delta_{ik} + a_{ni} a_{nl}\delta_{jk}) \\
+ 4k_1 J^{-1} \sum_{n=4,6} [2(I_n - 1)^2 k_2 + 1] \exp[k_2 (I_n - 1)^2] a_{ni} a_{nj} a_{nk} a_{nl},
\]

(3.27)

where we have used \( a_{ni}, n = 4, 6, i = 1, 2, 3, \) is the \( i \)th component of \( \mathbf{a}_n = \mathbf{F} \mathbf{a}_{0n}. \)

For the HGO-C model the stress is given by equations Equation (3.8) and Equation (3.9). Once again the isotropic contributions to \( c_{ijkl} \) are given by equations Equation (3.25) and Equation (3.26). The anisotropic contribution to \( c_{ijkl} \) for the HGO-C model is given as:

\[
(\sigma_{\text{aniso}})_{ij}\delta_{kl} + \frac{\partial(\sigma_{\text{aniso}})_{ij}}{\partial F_{\kappa\alpha}} F_{\kappa\alpha} = 4k_1 J^{-1} \sum_{n=4,6} [1 + 2k_2 (\bar{T}_n - 1)^2] \exp[k_2 (\bar{T}_n - 1)^2] \\
\times (\bar{\sigma}_{ni}\bar{\sigma}_{nj} - \frac{1}{3} \bar{T}_n \delta_{ij}) (\bar{\sigma}_{nk}\bar{\sigma}_{nl} - \frac{1}{3} \bar{T}_n \delta_{kl}) \\
+ 2k_1 J^{-1} \sum_{n=4,6} (\bar{T}_n - 1) \exp[k_2 (\bar{T}_n - 1)^2] (\delta_{ik}\bar{\sigma}_{nj}\bar{\sigma}_{nl} + \delta_{jk}\bar{\sigma}_{ni}\bar{\sigma}_{nl} \\
- \frac{2}{3} \delta_{kl}\bar{\sigma}_{ni}\bar{\sigma}_{nj} - \frac{2}{3} \delta_{ij}\bar{\sigma}_{nk}\bar{\sigma}_{nl} + \frac{2}{3} \bar{T}_n \delta_{ij} \delta_{kl}),
\]

(3.28)

where \( \bar{\sigma}_{ni} \) is the \( i \)th component of \( \mathbf{\bar{\sigma}}_n = \mathbf{F} \mathbf{a}_{0n}. \)
Bibliography


On the correct interpretation of measured force and calculation of material stress in biaxial tests

Abstract

Biaxial tests are commonly used to investigate the mechanical behaviour of soft biological tissues and polymers. In the current paper we uncover a fundamental problem associated with the calculation of material stress from measured force in standard biaxial tests.

In addition to measured forces, localized unmeasured shear forces also occur at the clamps and the inability to quantify such forces has significant implications for the calculation of material stress from simplified force-equilibrium relationships. Unmeasured shear forces are shown to arise due to two distinct competing contributions: (1) negative shear force due to stretching of the orthogonal clamp, and (2) positive shear force as a result of material Poisson-effect. The clamp shear force is highly dependent on the specimen geometry and the clamp displacement ratio, as
consequently, is the measured force-stress relationship.

Additionally in this study we demonstrate that commonly accepted formulae for the estimation of material stress in the central region of a cruciform specimen are highly inaccurate. A reliable empirical correction factor for the general case of isotropic materials must be a function of specimen geometry and the biaxial clamp displacement ratio. Finally we demonstrate that a correction factor for the general case of non-linear anisotropic materials is not feasible and we suggest the use of inverse finite element analysis as a practical means of interpreting experimental data for such complex materials.

4.1 Introduction

Biaxial testing is commonly used to investigate the mechanics of anisotropic soft tissues and polymers. Typically the goal of such tests is to determine the material stress-strain behaviour from measured forces and displacements.

The experimental measurement of strain at a central region of interest (ROI) in biaxial tests, using methods such as digital image correlation (DIC), has been well established (Humphrey et al., 1990b; Lyons et al., 2014). The use of ultrasound speckle tracking has been employed for even more accurate measurement of specimen deformation (Perez et al., 2014). Hence measurement of strain is not the focus of this paper. However, a rigorous analysis of commonly used methodologies for stress calculation from experimentally measured force has not been performed. In the current paper we highlight a fundamental problem in relating material stress to experimentally measured load-cell force, demonstrating that this relationship is non-trivial for biaxial tests. We demonstrate that the material stress in cruciform specimens cannot be trivially determined by dividing the load-cell force by a cross-sectional area (Simón-Allué et al., 2014; Pancheri et al., 2014; Waldman and Lee,
In biaxial tests two methods are commonly used to attach test specimens to the machine actuators. They are either held rigidly in clamps (Waldman and Lee, 2005), or anchored with rotating rakes/sutures (Humphrey et al., 1990a). The difficulties associated with sutured specimens have been highlighted previously. Uniformity of the strain field (and consequently the stress field) is highly sensitive to the number of suture attachment points, the regularity of their spacing and alignment (Eilaghi et al., 2009). This leads to stress concentrations extending within the perceived ROI of uniform stress (Sacks, 2000). Additionally, it is unclear whether there is full recruitment of collagen fibres throughout the specimen when sutures are used (Billiar and Sacks, 1997, 2000; Waldman et al., 2002). Due to the aforementioned deficiencies of suture based attachment, this paper focuses on the use of rigidly clamped specimens for biaxial tests.

The use of an empirical correction factor to increase the accuracy of the standard methodology for stress calculation has been proposed by Jacobs et al. (2013). However, the reliability and general applicability of such a correction factor over a range of specimen geometries and boundary conditions has not been examined, and a physical basis for a correction factor has not been established.

Recent papers in the field of composite materials have suggested modifications to specimen geometries to overcome difficulties in interpreting biaxial test results. These range from the milling of a reduced cross-sectional area in the centre of the specimen (Smits et al., 2006) to the inclusion of holes and angled slots in the test specimen (Schmaltz and Willner, 2014). However such modifications are unsuitable for testing of soft tissues.

The current paper is structured as follows. Section 4.3 examines the net forces in a cruciform specimen under biaxial tension and shows that localised unmeasured shear forces at the clamps prohibit direct calculation of stress from the measured
force. An analytical model is used to uncover the effect of two distinct and competing components of the unmeasured shear force. The significance of such localised shear forces on the accurate calculation of material shear stress is demonstrated. Section 4.4 focuses on commonly accepted formulae used to calculate stress from experimentally biaxial data. It is demonstrated that such methods will yield errors ranging from 30-50%. In Section 4.5 we establish that a correction factor for biaxial testing of isotropic materials must be a function of specimen geometry and the biaxial clamp displacement ratio. Finally we demonstrate that a correction factor for the general case of non-linear anisotropic materials is not feasible and we suggest the use of inverse finite element analysis as a practical means of interpreting experimental data for such complex materials.

4.2 Methods: Finite element model implementation

Figure 4.1A shows the typical set-up for a biaxial test of a cruciform specimen (see experimental studies of Waldman and Lee (2005); Lecompte et al. (2007); Simón-Alluè et al. (2014)). The specimen arms are held rigidly in clamps and fixed displacements, $u_x$ and $u_y$, are applied to Clamp-$x$ and Clamp-$y$ respectively. Load-cells in series with the clamp actuators measure the reaction forces $F_x$ and $F_y$, in the direction of applied displacement at Clamp-$x$ and Clamp-$y$ respectively.

Considering material and geometric symmetry, a three-dimensional finite element (FE) mesh of half a specimen is constructed (see Figure 4.1B). Figure 4.1B also illustrates the boundary conditions, applied clamp displacements, and resultant reaction forces, as well as the geometric parameters $w_0$ and $l_0$ used for the model (in the absence of material symmetry in the stretching axis, the full specimen geometry must be modelled as detailed in Appendix B). A range of specimen geometries is considered whereby the arm width to arm length ratio $w_0/l_0$ is varied. Addi-
Figure 4.1: A) Schematic of the specimen geometry and applied boundary conditions for biaxial test investigation. Displacements $u_x$ and $u_y$ at the clamps, as shown. Forces $F_x$ and $F_y$ are measured by load cells, as indicated. B) Half-specimen geometry used for the FE model (assuming material symmetry), outlining the geometric parameters $w_0$ and $l_0$, and the section line A–A (through the centre of the specimen).
tionally a range of clamp displacement ratios \( u_y/u_x \) is considered, with a reference displacement of \( u_x^{max}/l_0 = 0.2 \) being applied at Clamp-x in all cases.

FE simulations are performed using the Abaqus/Standard (v6.13-2, DS Simulia, R.I., U.S.A.) software package. The geometry is meshed using hexahedral elements each with eight integration points. Between 58,885 and 153,860 elements are used depending on the geometry in question. A mesh sensitivity study revealed that a converged solution is obtained for the mesh densities quoted above.

Simulations are performed using both isotropic and anisotropic constitutive models. A neo–Hookean constitutive model is used to simulate an isotropic material (see Equation (4.1)), with a shear modulus \( \mu = 7.0 \) kPa and a bulk modulus \( \kappa = 60.0 \) kPa. These values are taken from a recent study of the ground matrix material in arterial tissue (Nolan and McGarry, 2015). An anisotropic material is simulated using a compressible version of the constitutive model by Holzapfel et al. (2000), previously reported by Nolan et al. (2014) (see Equation (4.2)). This formulation is implemented in an Abaqus UMAT. Two families of fibres are defined in the \( x-y \) plane, symmetrically arranged at \( \pm 30.0^\circ \) to the \( x \)-axis, with material parameters \( \mu = 7.0 \) kPa, \( \kappa = 60.0 \) kPa, \( k_1 = 2.0 \) kPa, \( k_2 = 2.0 \). These values are based on the experimental work of (Nolan and McGarry, 2015).

\[
\sigma_{iso} = \kappa(J - 1) \mathbf{I} + \frac{\mu}{J^{5/3}} \left( b - \frac{1}{3} J_1 \mathbf{I} \right) \tag{4.1}
\]

\[
\sigma_{aniso} = \sigma_{iso} + \frac{2k_1}{J} \sum_{i=4,6} (I_i - 1) \exp \left[ k_2 (I_i - 1)^2 \right] (\mathbf{a}_i \otimes \mathbf{a}_i) \tag{4.2}
\]

In Equations (4.1) and (4.2) \( J \) is the determinant of the deformation gradient \( \mathbf{F} \),
Figure 4.2: Plot of the ratio of the integrated normal stress on A–A to the measured clamp force, as a function of specimen arm width to arm length ratio for an isotropic material. Results are presented for three different clamp displacement ratios, $u_y/u_x$. In general the integrated stress is not equal to the measured clamp force and is dependent on specimen geometry and clamp displacement ratio. Note that where $u_y/u_x = 0.0$ the position of Clamp-$y$ is kept fixed and Clamp-$x$ is displaced up to $u_x^{\text{max}}/l_0$.

$b = FF^T$ is the left Cauchy-Green deformation tensor and $C = F^TF$ is the right Cauchy-Green deformation tensor. The first invariant $I_1$ is the trace of $b$, $I$ is the identity tensor, $I_i$ ($i = 4, 6$ when two fibre families are present) is the anisotropic invariant defined as $I_i = a_{0i} \cdot (Ca_{0i})$ where $a_{0i}$ is a unit vector indicating the direction of fibre reinforcement and $a_i$ is the same vector in the deformed configuration given by $a_i = Fa_{0i}$.

4.3 Can standard biaxial force measurement be directly related to material stress?

First we present the previously unreported finding that measured force in the clamp direction is not equal to the integral of the $\sigma_{xx}$ component of material stress along
a section through the specimen centre. We demonstrate that this unexpected result emerges due to the complex geometry and boundary conditions employed in a standard biaxial test setup.

The Cauchy stress, $\sigma_{xx}$, normal to section A–A at the centre of the specimen is integrated over section A–A, $\iint_{A-A} \sigma_{xx} dydz$. Figure 4.2 plots the ratio of this integrated stress to the measured force $F_{x}^{\text{measured}}$ at Clamp-$x$ for a range of specimen geometries ($0.2 \leq w_0/l_0 \leq 0.9$) and clamp displacement ratios ($u_y/u_x = \{0.0, 0.5, 1.0\}$) where the material is modelled as isotropic. It is clear that the measured clamp force is not equal to the integral of the stress on section A–A. Furthermore the imbalance between clamp force and the integrated stress is dependent on both the specimen geometry and clamp displacement ratio. When the specimen has slender arms (low $w_0/l_0$) the integrated stress is larger than the clamp force; however, as the specimens become more square-like in geometry (high $w_0/l_0$) this relationship is reversed. Importantly, there is no single specimen geometry for which $\iint_{A-A} \sigma_{xx} dydz = F_x$ for all clamp displacement ratios. The influence of $\kappa/\mu$ and $u_x^{\text{max}}/l_0$ were also examined, but were found to be of secondary importance.

In order to explain this imbalance between the measured clamp force $F_x^{\text{measured}}$ and the integrated material stress $\iint_{A-A} \sigma_{xx} dydz$, Figure 4.3 presents a free-body diagram of the biaxial test setup considering all reaction forces in the $x$-direction. Of course $\iint_{A-A} \sigma_{xx} dydz$ must be equal to the net reaction forces in the $x$-direction. Figure 4.3 illustrates that the imbalance between the integrated stress and $F_x^{\text{measured}}$ is due to an unmeasured force in the $x$-direction at Clamp-$y$ (both top and bottom).

Hence $\iint_{A-A} \sigma_{xx} dydz = F_x^{\text{measured}} + 2F_x^{\text{unmeasured}}$, and in general $\iint_{A-A} \sigma_{xx} dydz \neq F_x^{\text{measured}}$. Standard biaxial test setups do not record the reaction force $F_x^{\text{unmeasured}}$ at Clamp-$y$; to do so would be technically challenging. Take for instance the simplest case of an isotropic material. $F_x^{\text{unmeasured}}$ is counteracted by an equal and opposite force on the left hand side of the centre-line on the free-body diagram in Figure 4.3.
Figure 4.3: Free-body diagram of the net forces in the $x$-direction in a cruciform specimen under biaxial tension. The force measured by Clamp-$x$ plus two unmeasured force components on Clamp-$y$ (top and bottom) are equal to the integral of the normal stress in the $x$-direction over the cross-sectional area along the centreline (section A–A). The objective of a biaxial test is to determine the Cauchy stress $\sigma_{xx}$; however, the unmeasured forces ($F_x^{\text{unmeasured}}$) prohibit the direct calculation of stress from the load-cell measured force ($F_x^{\text{measured}}$).
Hence the net force in the $x$-direction Clamp-$y$ is zero. To determine $F_{x}^{\text{unmeasured}}$ one would have to measure the force in the $x$-direction at several discrete points along Clamp-$y$. In fact in the absence of material symmetry (for example Appendix B) the distribution of $F_{x}^{\text{unmeasured}}$ at Clamp-$y$ is not symmetric and an additional moment occurs at the clamp.

An interesting feature of the result in Figure 4.2 is that the integrated stress is greater than the measured clamp force $F_{x}^{\text{measured}}$ when the cruciform arms are slender ($w_0/l_0 \rightarrow 0$), whereas this relationship is reversed when the geometry becomes more square-like ($w_0/l_0 \rightarrow 1$). This implies that the unmeasured force $F_{x}^{\text{unmeasured}}$ at Clamp-$y$ changes direction as the specimen geometry changes from a slender-armed cruciform to a square. This change in reaction force direction is evident from the positive shear stresses at Clamp-$y$ for a square-like specimen (Figure 4.4A), in contrast to the negative shear stresses at Clamp-$y$ for the slender-armed cruciform (Figure 4.4B).

In order to understand the dependence of the direction and magnitude of the unmeasured shear force at Clamp-$y$ on the specimen geometry, we now present an analytical solution for an idealised biaxial cruciform specimen. As shown in Figure 4.5, the deformation of the arm connecting Clamp-$y$ to the centre of the specimen can be decomposed into two distinct components for an idealised infinitesimal linear elastic analysis.

*Component (i)* - A negative reaction force develops at Clamp-$y$ as a direct result of the positive pulling-force imposed at Clamp-$x$. If the specimen geometry is more square-like (where $w_0/l_0 \rightarrow 1$) a large proportion of the pulling force at Clamp-$x$ ($F_{x}^{\text{measured}}$) is balanced by the unmeasured force at Clamp-$y$. In contrast, if the specimen has a slender-armed geometry (where $w_0/l_0 \rightarrow 0$) a very small proportion of the pulling force at Clamp-$x$ ($F_{x}^{\text{measured}}$) is balanced by the unmeasured force at Clamp-$y$. 
Figure 4.4: A) Contour plot of shear stress ($\sigma_{xy}$) in a square-like geometry ($w_0/l_0 = 0.8$). Note the presence of positive shear stress at the clamps and that the reaction force $F_{x\text{unmeasured}}$ acts in a negative direction. B) Contour plot of shear stress ($\sigma_{xy}$) in a slender-armed geometry ($w_0/l_0 = 1/3$). Note the presence of negative shear stress at the clamps and that the reaction force $F_{x\text{unmeasured}}$ acts in a positive direction in this case.
Figure 4.5: Schematic of an idealised analytical model of a biaxial test, assuming infinitesimal deformation and linear elasticity. The unmeasured reaction force at Clamp-$y$ results from two distinct and competing components of deformation. The negative reaction force $T_x^{(i)}$ due to Deformation Component $(i)$ arises due to an applied displacement $\alpha l_0$ of the orthogonal Clamp-$x$. The positive reaction force $T_x^{(ii)}$ due to Deformation Component $(ii)$ arises due to the Poisson-effect lateral contraction of the cruciform arm and the fixed-end boundary condition at Clamp-$y$. Linear superposition is used to determine the unmeasured force at Clamp-$y$ ($T_x^{UM} = T_x^{(i)} + T_x^{(ii)}$).
A schematic of the deformation caused by Component \((i)\) is outlined in Figure 4.5. It is expressed in terms of the undeformed co-ordinates \(X\) and \(Y\) by the following deformation gradient

\[
F = \begin{bmatrix}
1 + \frac{\alpha w_0 Y}{(l_0 - w_0) w_0} & \frac{\alpha w_0 X}{(l_0 - w_0) w_0} \\
0 & 1
\end{bmatrix}
\] (4.3)

The Green-Lagrange strain is defined as \(E = (1/2)(F^T F - I)\). The \(xy\) component of the strain is expressed as,

\[
E_{xy} = \frac{1}{2} \left\{ \frac{(\alpha w_0 X)(1 + \alpha w_0 Y)}{(l_0 - w_0)^2 w_0^2} \right\}
\] (4.4)

The shear strain deformation imposed at Clamp-\(y\) \((Y = 0)\) is then given as

\[
E_{xy} \bigg|_{Y=0} = \frac{1}{2} \left\{ \frac{(\alpha w_0 X)}{(l_0 - w_0)^2 w_0^2} \right\}
\] (4.5)

Therefore the force at Clamp-\(y\) due to Component \((i)\), \(T_x^{(i)}\), (normalized by the material shear modulus \(\mu\)) is obtained by integration of the shear strain along Clamp-\(y\).

\[
\frac{T_x^{(i)}}{\mu} = \int_0^{w_0} E_{xy} \bigg|_{Y=0} dX = \frac{\alpha w_0}{(l_0 - w_0)^2}
\] (4.6)

A plot of the normalized analytical Component \((i)\) force \(T_x^{(i)}/\mu\) at Clamp-\(y\) is shown in Figure 4.6A (black dashed line). As the ratio of \(w_0/l_0\) increases, so too does the magnitude of \(T_x^{(i)}\), i.e. more shear strain is imposed at Clamp-\(y\) for square-like specimens. If the specimen is slender-armed then \(w_0/l_0\) is small and as the cruciform
Chapter 4 140

Figure 4.6: A) Plot of the analytical reaction force components at Clamp-\(y\) as a function of specimen geometry: \(T_x^{(i)}\) the analytically derived shear-effect reaction force, \(T_x^{(ii)}\) the analytically derived Poisson-effect reaction force, and the sum of the two forces. B) The ratio of the integrated stress to the measured force is approximated by \(\xi_a = \left\{ \frac{(T_x^M - T_x^{UM})}{T_x^M} \right\}\). The resultant force imbalance is plotted for a clamp displacement ratio \(u_y/u_x = 0\) where \(T_x^{UM} = T_x^{(i)}\), and \(u_y/u_x = 1\) where \(T_x^{UM} = T_x^{(i)} + T_x^{(ii)}\). The plots are similar to the results shown in Figure 4.2 for large deformation non-linear FE simulations.

Arm width decreases \(T_x^{(i)} \to 0\).

**Component (ii):** In addition to Component (i) of the unmeasured force described above, if \(u_y/u_x \neq 0\) then stretching the cruciform arm attached to Clamp-\(y\) will result in lateral contraction of material in the arm due to the Poisson-effect. Figure 4.5 illustrates that rigid fixation at Clamp-\(y\) results in a localized prevention of lateral contraction resulting in an additional reaction force in the \(x\)-direction at Clamp-\(y\). This Component (ii) force (Poisson-effect reaction force), \(T_x^{(ii)}\), acts in the opposite direction to \(T_x^{(i)}\). A plot of the normalized force \(T_x^{(ii)}\), obtained using a semi-analytical numerical method (again for the idealized case of linear elastic infinitesimal deformation), is shown in Figure 4.6A (grey dashed line). In contrast to \(T_x^{(i)}\), the Poisson-effect force is present in slender-armed geometries and reaches its
maximum magnitude when \( w_0/l_0 \approx 0.45 \). After this the magnitude of \( T_x^{(ii)} \) decreases as the specimen geometry becomes more square-like.

The total unmeasured force (UM) at Clamp-y for this idealised linear elastic infinitesimal strain analysis can now be determined by superposition of Component (i) and (ii), \( T_x^{UM} = T_x^{(i)} + T_x^{(ii)} \). This is plotted in Figure 4.6A (solid black line). The direction of \( T_x^{UM} \) is dependent on the competition between Component (i) and Component (ii). For square-like specimens Component (i) dominates \( T_x^{UM} \), whereas for slender-armed specimens the contribution of Component (i) is significantly reduced and the Poisson-effect force, \( T_x^{(ii)} \), dominates with the result that \( T_x^{UM} \) is negative.

For the idealised deformation considered in Figure 4.5 and Equations (4.3)-(4.6) above, the measured force at Clamp-x is given as \( T_x^{M}/\mu = 3\alpha w_0 \) (assuming material incompressibility). In Figure 4.6B we plot the analytical force imbalance \( \xi_a = \{ (T_x^{M} - T_x^{UM})/T_x^{M} \} \) as a function of the specimen geometry (noting that this quantity is equivalent to \( \int_A \sigma_{xx} dydz/F_{x measured} \) plotted in Figure 4.2 for realistic finite deformation geometry). Firstly, we consider the force imbalance \( \xi_a \) for Component (i) only. For very long slender-armed specimens \( T_x^{(i)} \) is small and \( \xi_a \approx 1 \), whereas for square-like specimens \( T_x^{(i)} \) is large and \( \xi_a < 1 \). It should be noted that this result for Component (i) is equivalent to the case \( u_y/u_x = 0 \) previously considered in Figure 4.2. Clearly this idealised analytical model can explain the trend observed in the realistic large-deformation analysis for the case of \( u_y/u_x = 0 \) presented in Figure 4.2. The superimposition of the Poisson-effect force, \( T_x^{(ii)} \), in the analytical model explains the increase in \( \xi_a \) for equi-biaxial stretching \( u_y/u_x = 1 \), again displaying a remarkable similarity to the plot in Figure 4.2.

The idealised infinitesimal strain linear elastic analyses presented in Figure 4.6 provide a clear insight into the complex relationship between the measured force and material stress in biaxial testing. However biaxial testing of biological tissues and polymers generally entails non-linear material behaviour and large deformations.
Therefore the idealised analyses of Figure 4.6 do not provide accurate predictions, and non-linear finite element analyses of the type presented in Figure 4.2 are required.

It is important to note that problems highlighted in this section will occur regardless of choice of constitutive model.

4.4 Inaccuracy of standard methods for biaxial stress calculation

In this section we investigate the inaccuracy of the standard technique of dividing the measured force by a representative cross-sectional-area (CSA) to determine a stress state in the central region of a specimen. Several choices of CSA have been implemented in the literature. Here we demonstrate that none of the previously proposed CSAs (Pancheri et al., 2014; Robinson and Tranquillo, 2009; Simón-Allué et al., 2014) result in the accurate estimation of material stress at the centre of the specimen.

As soft-tissues are typically subjected to finite strains in biaxial tension tests, finite deformation continuum mechanics must be used to determine the Cauchy stress. The typical procedure (Humphrey et al., 1990a; Sacks, 2000) is to first compute the nominal/first Piola–Kirchhoff stress $\mathbf{P}$ using the experimentally measured forces and the undeformed specimen geometry. The Cauchy stress $\sigma$ is then calculated from the push-forward operation $\sigma = (1/J) \mathbf{FP}$. Soft tissues are commonly assumed to be incompressible, this implies that $J = 1$. In the absence of shear deformation the normal components of the deformation gradient are assumed to be equal to the principal stretch ratios, i.e. $F_{xx} = \lambda_x$ and $F_{yy} = \lambda_y$. The principal stretch ratios are measured either through change of a gauge length, or a strain map obtained from DIC. Combining the above equations, the Cauchy stress components may be
Figure 4.7: A) Schematic showing the CSAs used to calculate stress in Equation (4.7). B) Plot of the normal stress $\sigma_{xx}$ along the centreline A–A, normalised by the shear modulus $\mu$, for an isotropic material. The specimen has geometry $w_0/l_0 = 1/3$ and is subjected to equi-biaxial stretch, $u_y/u_x = 1$. The non-uniformity of the stress in the material is clear. The stress calculated using Equation (4.7) and CSA widths $l_0$, $w_0$, and $b_0$ are superimposed on the plot. Using the cruciform arm width, $w_0$ or the side of the largest square that can fit inside the specimen $b_0$ for the CSA leads to an overestimation of stress. Using the arm length $l_0$ results in an underprediction of material stress at the centre of the specimen. C) Plot showing results for an anisotropic material. Again the stress calculated using Equation (4.7) results in substantial errors.

The normal stress is determined using the formulae,

$$
\sigma_{xx} = \frac{\lambda_x F_x}{A_0}; \quad \sigma_{yy} = \frac{\lambda_y F_y}{A_0},
$$

where $A_0$ is the representative undeformed CSA. However, in Equation (4.7) there are two implicit assumptions. Firstly, the normal stress throughout the CSA must be homogeneous. Secondly, the stress biaxiality throughout the CSA must be uniform (i.e. that $\sigma_{xx}/\sigma_{yy} = \text{constant}$). We now investigate commonly assumed CSAs for cruciform specimens and whether the above criteria are fulfilled.

Figure 4.7B plots the normal Cauchy stress $\sigma_{xx}$ on section A–A for an isotropic specimen under equi-biaxial stretch. Firstly it is clear there is a non-uniform stress
distribution along this section line. Even within the central region the $\sigma_{xx}$ stress at $x = 0, y = w_0$ is 28% less than that at the centre-point. Regardless of whether one considers the entire section A–A or the region between $\pm w_0$, the criterion of stress homogeneity has not been met.

Figure 4.7A shows the different representative CSAs found in the literature: $w_0$ (Robinson and Tranquillo, 2009), $l_0$ (Eng et al., 2014), or the side of the largest square which can be drawn inside the specimen $b_0$ (Simón-Allué et al., 2014). In Figure 4.7B we have superimposed the stress that is calculated using Equation (4.7), and these different CSAs. The undeformed thickness $t_0$ is used in all cases. None of the CSAs result in an accurate estimate of the stress at the centre of the specimen. The cross-sectional widths $b_0$ and $w_0$ overestimate the stress by 32% and 43% respectively, while using $l_0$ underestimates the stress by 52%.

Figure 4.7C repeats the above procedure for the anisotropic material outlined in Section 4.2 As with the isotropic material, non-uniformity of the stress on section A–A is observed. The stress $\sigma_{xx}$ is 19.5% less at $w_0$ than at the centre-point, again demonstrating that significant stress inhomogeneity exists even between $\pm w_0$. The use of various different cross-section widths has similarly poor results to the isotropic case. The use of $b_0$ and $w_0$ overestimates the stress at the centre-point by 40% and 52%, respectively, while $l_0$ underestimates the stress at the centre-point by 49%.

The next condition which must be met to ensure the validity of Equation (4.7) is that the biaxiality of the stress ($\sigma_{xx}/\sigma_{yy}$) in the specimen must be constant on the representative CSA. Figure 4.8A plots the stress biaxiality in an isotropic specimen under equi-biaxial stretch, $u_y/u_x = 1$. The biaxiality of the stress is inhomogeneous along any representative CSA, and throughout the specimen in general. For the case of an equi-biaxial stretch in Figure 4.8A one might expect $\sigma_{xx} = \sigma_{yy}$ in the central region of the specimen between $\pm w_0$, however this is true only at the centre-point of the specimen $(x, y) = (0, 0)$. Figure 4.8B plots the biaxiality of the stress in the
Figure 4.8: A) Contour plot of the stress biaxiality ($\sigma_{xx}/\sigma_{yy}$) in an isotropic specimen where $w_0/l_0 = 1/3$ under equi-biaxial stretch ($u_y/u_x = 1$). Note that the stress biaxiality is inhomogeneous throughout and that $\sigma_{xx} = \sigma_{yy}$ at one point only, the centre-point of the specimen. The ratio of the measured force at the clamp $F_x/F_y = 1$. B) Contour plot of the stress biaxiality ($\sigma_{xx}/\sigma_{yy}$) in an anisotropic specimen with $w_0/l_0 = 1/3$ under equi-biaxial stretch ($u_y/u_x = 1$). Note that the stress biaxiality is inhomogeneous throughout the specimen and the ROI. The stress biaxiality at the centre of the specimen $\sigma_{xx}/\sigma_{yy} = 1.98$ whereas the ratio of the measured force at the clamp $F_x/F_y = 1.58$. Results are plotted in the undeformed configuration.
anisotropic material. Again the biaxiality of the stress is inhomogeneous throughout the specimen.

A CSA cannot be defined where $\sigma_{xx}/\sigma_{yy} = \text{constant}$, on this basis alone Equation (4.7) cannot be used to compute stress in a cruciform specimen. Furthermore, for isotropic specimens the ratio of $\sigma_{xx}$ to $\sigma_{yy}$ is equal to the ratio of the measured forces $F_x$ to $F_y$ only at a single point in the specimen. However, for an anisotropic specimen the stress ratio cannot be related to the measured force ratio at any point in the specimen. Hence, the biaxiality of the stress state or the degree of material anisotropy cannot be simplistically inferred from the ratio of the measured clamp forces $F_x/F_y$.

As a final note on computed stress biaxiality, von Mises stress is commonly used to characterise material stress in computational studies on biaxial testing (Jacobs et al., 2013; Sun et al., 2005). In Appendix A it is shown that von Mises stress gives a misleading indication of stress homogeneity.

In conclusion, it is apparent that simple formulae such as Equation (4.7) are incapable of accurately calculating the material stress in a cruciform specimen, regardless of choice of CSA.

### 4.5 Can simple correction factors be established to improve the accuracy of current standard methods of stress estimation?

In Section 4.4 we have demonstrated that standard formulae which divide force by a representative CSA do not provide an accurate and reliable estimate of material stress during a biaxial test. In this section we attempt to establish empirical correction factors, for an isotropic neo–Hookean material, that can be used to improve the direct prediction of material stress from measured force. We demonstrate that the
determination of such correction factors is a complex multi-variable problem which becomes unmanageable for an anisotropic material. It is proposed that an inverse FE algorithm is best suited to determine material stress in an anisotropic material.

Here we consider the simplest case of an isotropic material. Given the inhomogeneous stress state in the central region of a specimen (see Figure 4.7), we focus on the identification of correction factors for the centre-point of the specimen. Recall that for isotropic materials the biaxiality of the stress is equal to the ratio of the clamp displacements and the measured clamp force; $\sigma_{xx}/\sigma_{yy} = u_x/u_y = F_x/F_y$. As a starting point, based on previous approaches to the problem (see Equation (4.7)), we define the “apparent stress” $\hat{S}_{xx}$ as

$$\frac{\sigma_{xx}}{\hat{S}_{xx}} = \frac{\lambda x F_x}{w_0 l_0}$$  \hspace{1cm} (4.8)
In Figure 4.9 we plot the ratio of the computed Cauchy stress at the centre-point to the apparent stress \( \frac{\sigma_{xx}}{\hat{S}_{xx}} \) for a range of specimen geometries \((0.2 \leq w_0/l_0 \leq 0.9)\) and clamp displacement ratios \((u_y/u_x = \{0.0, 0.5, 1.0\})\), determined using FE analysis. Figure 4.9 shows that as \( u_y/u_x \) increases, so too does the deviation of the real material stress from the apparent stress. This is due to the increasing influence of the Poisson-effect force on the stress state, as demonstrated in Section 4.3. These data are used to determine an empirical correction factor \( C \) which may be used to calculate the Cauchy stress \( \sigma_{xx} \) at the centre-point of a cruciform specimen from the apparent stress \( \hat{S}_{xx} \), such that

\[
\sigma_{xx} = C \hat{S}_{xx}
\]

Assuming a polynomial function, the correction factor \( C \) is found to be cubic in \( w_0/l_0 \), quadratic in \( u_y/u_x \), and is given as

\[
C = a \left( \frac{w_0}{l_0} \right)^3 + b \left( \frac{w_0}{l_0} \right)^2 + c \left( \frac{w_0}{l_0} \right)^2 \left( \frac{u_y}{u_x} \right) + d \left( \frac{u_y}{u_x} \right)^2 + e \left( \frac{w_0}{l_0} \right) \left( \frac{u_y}{u_x} \right) + f \left( \frac{w_0}{l_0} \right) + g \left( \frac{u_y}{u_x} \right) + h \tag{4.9}
\]

The constants for Equation 4.9 are given in Table 4.1. This polynominal fit has a correlation coefficient \( r^2 = 0.99 \) and root-mean-square error of \( 6.8 \times 10^{-3} \). The correction factor is independent of the clamp displacement \( u_x/l_0 \) for a perfectly linear material, and this parameter is found to be negligible for a quasi-linear isotropic neo–Hookean material. Similarly, for a linear elastic material, the correction factor is independent of the material stiffness, and for a quasi-linear elastic material the

<table>
<thead>
<tr>
<th></th>
<th>a</th>
<th>b</th>
<th>c</th>
<th>d</th>
<th>e</th>
<th>f</th>
<th>g</th>
<th>h</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>-1.263</td>
<td>1.562</td>
<td>0.05395</td>
<td>0.04474</td>
<td>0.08011</td>
<td>-0.5683</td>
<td>-0.1841</td>
<td>0.863</td>
</tr>
</tbody>
</table>

Table 4.1: Table of constants for Equation (4.9) which may be used to determine an empirical correction factor to calculate stress at the centre-point in an isotropic specimen.
material parameters are found to be negligible. For an isotropic material, due to symmetry, one need only examine clamp displacement ratios \( 0 \leq u_y/u_x \leq 1 \).

Clearly an empirical correction factor for a simple neo-Hookean isotropic material is a highly non-linear function of the specimen geometry and the applied clamp displacement ratio. The complexity of the problem is substantially increased for anisotropic materials, for which the following factors must be taken into account:

1. In general the biaxiality of the stress \( \sigma_{xx}/\sigma_{yy} \) for anisotropic materials does not equal the clamp displacement ratio \( u_x/u_y \) nor does it equal the measured clamp force \( F_x/F_y \). Consequently \( \sigma_{xx}/\sigma_{yy} \neq \dot{S}_{xx}/\dot{S}_{yy} \) and to establish a correction factor, the relationship between these two ratios must be determined as a function of the degree of material anisotropy. This is another variable which must be included in any proposed correction factor. The degree of anisotropy in a specimen of biological tissue is generally not known \textit{a priori}, and its characterisation is typically one of the primary objectives of biaxial tension tests.

2. In the case of highly non-linear materials (e.g. arterial tissue) the ratio \( \sigma_{xx}/\dot{S} \) will be highly dependent on the magnitude of applied stretch \( u_x/l_0 \), in addition to the clamp displacement ratio \( u_y/u_x \). Additionally the degree of material non-linearity is relevant thus adding a further two variables to any proposed correction factor. Once again we are confronted with the issue that the degree of material non-linearity is not known \textit{a priori} and is an objective of the experiment.

3. Due to the absence of material symmetry, experiments/simulations should be performed for the range \( 0 \leq u_x/u_y \leq 1 \) in addition to \( 0 \leq u_y/u_x \leq 1 \).

Any proposed correction factor must therefore be a function of the following four
The calculation of a general correction factor that accounts for a wide range of material non-linearities and a wide range of material anisotropy is therefore not feasible. A far more practical solution is provided by an inverse FE calibration of specific experimental data to determine material stress distribution and to calibrate and validate a constitutive law. This method entails picking a constitutive model for the material being tested, performing simulations which replicate the experimental protocol, and iterating upon the material parameters in the constitutive law until the experimental data is satisfactorily matched. The appropriateness of the assumed constitutive law is established by the goodness-of-fit of the predicted behaviour for the optimized material properties. If the initially assumed constitutive law is not appropriate for the anisotropic material then an accurate replication of the experimental data will not be achieved by the inverse FE approach, and the process must be repeated using an alternative constitutive law. The procedure for inverse FE analysis is outlined in Appendix B, and the accurate interpretation of experimental data using this methodology is outlined in detail in a companion paper (Nolan and McGarry, 2015). Most importantly, the inverse FE method overcomes the issues relating to unmeasured forces and stress inhomogeneity outlined in Sections 4.3 and 4.4 of this paper. It is critically important, based on the findings of the current study, that inverse FE methodologies entail the comparison of computed clamp reaction forces (not the computed material stress) with measured clamp reaction forces.

Furthermore, the inverse FE approach may be use in conjunction with experimental strain measurements using DIC (Lecompte et al., 2007). The advantage being that in-plane shear may be quantified using DIC (see Appendix B) and the
material parameters may be adjusted accordingly. For example in the anisotropic model described in Section 2 the fibre angles may be adjusted such that they are not symmetric about the $x$-axis.

### 4.6 Concluding remarks

In the current paper we uncover fundamental problems associated with biaxial tension tests on cruciform specimens.

(i) Firstly, that standard biaxial tests using cruciform specimens do not measure shear force at the clamps. Such unmeasured shear forces arise due to two distinct contributions: (1) negative shear force due to stretching of the orthogonal clamp, and (2) positive shear force as a result of material Poisson-effect. Due to the absence of experimental information on such unmeasured shear forces, the material stress cannot be directly related to the measured biaxial forces.

(ii) Secondly, standard formulae for the estimation of biaxial material stress in the central region of a cruciform specimen are highly inaccurate. The level of error is dependent on the specimen geometry, and clamp displacement ratio. A robust correction factor is proposed for isotropic materials. However, constitutive law calibration for anisotropic, non-linear materials can only be achieved by performing rigorous inverse FE analysis.

Key-point (i) above is previously unreported for biaxial testing, yet its implications are highly significant for the interpretation of experimental data. For example, this offers a cogent explanation for the ostensibly inconsistent experimental results of Waldman and Lee (2005), where a different stress-strain relationship is reported for a square-like and slender-armed cruciform geometry. This geometry-specific discrepancy in material properties can be understood as follows. The unmeasured shear
clamp forces for square-like specimens are negative, therefore the measured force required to produce a given material stress will be overestimated. Hence an artificially high stress will be calculated using the incorrect commonly used formulae for force-stress conversion. On the other hand for slender-armed specimens the negative (Contribution (i)) force is reduced and the positive Poisson-effect force (Contribution (ii)) will become significant. Therefore the unmeasured force $F_{x}^{\text{unmeasured}}$ will result in the calculation of lower material stress and stiffness than the square-like specimen, and may underestimate the material stiffness if Contribution (ii) exceeds Contribution (i). The reader is referred to Figure 4 in Waldman and Lee (2005) for direct experimental evidence of the importance of Point (i) above.

The findings of the current paper are also relevant to biaxial testing where the specimen is clamped using sutures or rakes. As shown in Appendix C, biaxial deformation results in a rotation of the rakes, which can result in a significant unmeasured $x$-component of force at Clamp-$y$ (load-cell-$y$). Of course, similar to the rigidly clamped cruciform specimens, rake/suture anchored biaxial tests also require a detailed inverse FE analysis in order to relate measured force to material stress. This preliminary analysis is merely intended to motivate a more detailed finite element analysis of unmeasured shear forces for alternative clamping systems. Analyses should include the effect of finite deformation, stress concentration at the points of rake insertion, and evolution of the non-alignment of rake attachment points at large stretches. Additionally, technical experimental difficulties have previously been reported for suture/rake attached specimens (Eilaghi et al., 2009; Waldman et al., 2002).

In relation to key-point (ii) above, we demonstrate that the widely used “measured force/area” approach (see for example Eng et al. (2014); Robinson and Tranquillo (2009); Simón-Allué et al. (2014)) to calculating material stress in biaxial tests results in highly significant errors ranging from 32% to 52% depending on the
assumed CSA. A previous study (Jacobs et al., 2013) uses a constant correction factor for the direct calculation of measured stress from clamp force. However, in the current study we demonstrate that a reliable correction factor for the general case of isotropic materials must be a function of specimen geometry and the biaxial clamp displacement ratio. A constant correction factor, as proposed by Jacobs et al. (2013), will be appropriate for only one single specific specimen geometry with one single specific clamp displacement ratio. In contrast, here we perform an extensive parametric study in order to establish a reliable correction factor that can be generally applied to the biaxial testing of isotropic materials for a wide range of specimen geometries and clamp displacement ratios. In the case of anisotropic materials, we demonstrate that an empirical expression to relate measured force to material stress will be a highly non-linear function of four non-dimensional variables. The establishment of a general correction factor that accounts for a range of material non-linearity and a range of anisotropy levels would require a parametric study consisting of an unfeasible number of simulations (of the order of $10^3$). Therefore, we propose the inverse finite element analysis of case specific experimental data as the only practical means of correctly interpreting experimental data for non-linear anisotropic materials.

**Acknowledgements**

DRN wishes to acknowledge the receipt a PhD scholarship from the Irish Research Council and the College of Engineering and Informatics at NUI, Galway. We wish to thank Noel Reynolds for insightful discussions. This research was also funded under Science Foundation Ireland project SFI-12/IP/1723.
4.7 Appendices

Appendix 4A: Limitations of von Mises stress in the analysis of biaxial tests

It should be noted that only normal stress components are used to describe stress in the current study. Previous studies have used von Mises stress
\[ \sigma_{\text{Mises}} = \sqrt{\sigma_{xx}^2 - \sigma_{xx}\sigma_{yy} + \sigma_{yy}^2 + 3\sigma_{xy}^2} \] in plane stress) to characterise the stress in biaxial tests (Sun et al. (2005); Jacobs et al. (2013)). Figure 4.A.1A plots the normal stresses (\(\sigma_{xx}\) and \(\sigma_{yy}\)), and the von Mises stress (\(\sigma_{\text{Mises}}\)) along section A–A between \(-w_0\) and \(w_0\) for an equi-biaxial stretch of a slender-armed cruciform specimen (\(w_0/l_0 = 1/3\)). Once again it is apparent that the normal stresses are non-uniform within this section. The stress \(\sigma_{xx}\) decreases with increasing distance from the centre-point, while \(\sigma_{yy}\) increases with increasing distance from the centre-point.

Interestingly, von Mises stress is uniform along the ROI. An inspection of the equation for von Mises stress above explains why this is so. As we move away from the centrepoint, the decrease in \(\sigma_{xx}\) is matched by a corresponding increase in \(\sigma_{yy}\), leading to the calculation of a uniform von Mises stress. Figure 4.A.1B is a contour of normalised von Mises stress. It shows that von Mises stress is approximately uniform throughout significant portions of the centre of the specimen.

Finally, Figure 4.A.2 plots the normal stress \(\sigma_{xx}\) and the von Mises stress in both an isotropic and anisotropic material on section A–A. In both materials the von Mises stress appears to be significantly more homogeneous in the ROI than is the case.

It is clear that von Mises stress does not provide a meaningful representation of stress homogeneity or biaxiality (\(\sigma_{xx}/\sigma_{yy}\)). A previous study (Jacobs et al., 2013) proposed empirical correction factors to the relate von Mises stress at the ROI to
Figure 4.A.1: A) Plot of the normal stresses ($\sigma_{xx}$, $\sigma_{yy}$) and the von Mises stress along section A-A in the ROI for a specimen with geometry $w/l_0 = 1/3$ under an equi-biaxial stretch ($u_y/u_x = 1$). Stresses are normalised by the shear modulus $\mu$. B) Contour plot of the von Mises stress in the specimen normalised by the von Mises stress at the centre-point (CP). Note that $\sigma_{Mises}/\sigma_{Mises}^{CP} \approx 1$ throughout significant portions of the ROI.
Appendix 4B: Inverse finite element method to determine material behaviour

The inverse FE procedure involves the iterative simulation of an experiment using FE analysis to solve for the material parameter set that matches the experimental data. Inverse FE analysis is an optimization/minimization problem. An objective function $f(\Lambda)$ is established where $\Lambda$ is a material parameter set that defines the constitutive model in the FE simulation. If $f(\Lambda) = 0$ then the experimental data and FE simulation are identical.

The procedure is outlined in Figure 4.B.1. In the specific case of biaxial testing of cruciform specimens, we may use the experimentally measured clamp force-displacement curves and strain obtained from DIC to form the objective function. The objective function consists of two parts. The first part is the FE simulation of the biaxial tests, replicating the geometry and boundary conditions of the experiments. Simulations are performed for each displacement ratio examined ($n_{tests}$).
Figure 4.B.1: Flowchart outlining the iterative inverse FE method used to determine material properties. An initial guess of the material properties is made for the first iteration \((n = 1)\). The objective function \(f(\Lambda)\) is evaluated. This is a two step process, firstly FE simulations are performed for each experimental test. Secondly the clamp force-displacement curves from the FE simulations are compared to the experimental curves using a least-squares regression. Additionally the strain along a line from the FE simulation is compared to the strain in the specimen obtained using DIC. The objective function for that parameter set is computed using the sum of the \((1 - r^2)\) values. If the objective function satisfies the convergence criteria then the operation is terminated and the best-fit material parameters have be obtained. Otherwise a derivative free method is used to compute a new parameter set.
Figure 4.B.2: Contour plot of the $\varepsilon_{xx}$ component of the log strain an equi-biaxial stretch test on a anisotropic material with an offset axis of $\alpha = -20^\circ$. Note the asymmetry of the strain field.
For each simulation, net force-displacement curves at the $x$ and $y$ clamps are computed ($n_{clamps}$). The second part quantifies how closely the FE simulation reproduces the experimental data. A least-squares regression is calculated comparing the experimental and FE force-displacement curves. The strain along section A–A from $-w_0$ to $w_0$ from the FE simulation is compared to the strain obtained from DIC and a least-squares regression is calculated. The correlation coefficient $r^2$ is computed in each of these cases. As the correlation improves $r^2 \rightarrow 1$; $(1 - r^2)$ quantifies the goodness of fit. The objective function then is the sum of the goodness of fit measures, for the $n^{th}$ iteration,

$$f(\Lambda^{(n)}) = \sum_{i=1}^{nratio} \sum_{j=1}^{naxes} \sum_{k=1}^{ndic} (1 - r^2),$$ (4.B.1)

where $nratio$ are the number of unique displacement ratios used in the biaxial testing, $naxes$ are the number of axes the material is tested in, and $ndic$ are the number of DIC tests used. Convergence is judged to have occurred when the change in $f(\Lambda)$ is less than a predefined tolerance value. If convergence does not occur, a derivative-free, Nelder-Mead simplex algorithm is used to determine the next parameter set $\Lambda^{(n+1)}$ that should be evaluated by the objective function.

For the inverse FE method to be effective, it is critical that the chosen constitutive model can adequately capture the non-linearity and anisotropy of the material tested.

Figure 4.B.2A is a schematic showing the orientation of anisotropic fibres in a specimen. The principal material axis may be offset from the geometric axis by an angle $\alpha$. When $\alpha \neq 0^\circ$ then symmetry boundary conditions are invalid and the full geometry of the specimen must be modelled. Such a situation will lead to net moments at the clamps leading to asymmetric stress at the clamp. However such
moments are not measured experimentally, and the axial forces give no indication of this asymmetry. Figure 4.B.2B presents the $\varepsilon_{xx}$ component of the log strain in a materially anisotropic (Equation (4.2)) specimen with an offset angle $\alpha = -20^\circ$. The material orientation asymmetry is apparent. Fibre orientations are generally not known a priori, hence the incorporation of DIC measurements of strain into an inverse FE scheme are an effective way of capturing and accounting for material asymmetry.

Appendix 4C: Preliminary analysis of unmeasured shear forces in rake/suture anchored biaxial tests

Consider $N$ number of rakes attached to clamp-\textit{y} during an equi-biaxial deformation. The total measured force in the $y$-direction is given as $T_{y\text{measured}} = \sum_{i=1}^{N} T_{y}^{(i)}$. Similarly, the total unmeasured $x$-component of force at clamp-\textit{y} is given as $T_{x\text{unmeasured}} = \sum_{i=1}^{N} T_{x}^{(i)}$. As a preliminary analysis we consider a simplified case where (i) equal tension is assumed in the $N$ rakes along an edge, (ii) the $x$-displacements of the $N$ rakes attached to clamp-\textit{y} increase linearly from the centre-edge towards the corner of a square specimen, (iii) rake attachment points remain horizontally aligned during deformation. The dependence of the imbalance between measured $y$-force and unmeasured $x$-force is shown as a function of rake length in Figure C.1B for a range of applied equi-biaxial stretch magnitudes. The effect of rake length on force imbalance follows a similar trend to the effect of the arm-length for rigidly clamped cruciform specimens (see Figures 4.2 and 4.6). This result suggests that the force imbalance can be significant at high levels of specimen deformation, even if the rake length is significantly larger than the specimen length. It should be noted that, given the aforementioned simplifying assumptions, the relationships presented Figure C.1B merely demonstrate that the key points of the
Figure 4.C.1: A) Schematic of a biaxial specimen anchored with sutures/rakes. When the specimen is deformed to a strain $\alpha$, the rakes rotate incurring an $x$-component of force $T_x^{\text{unmeasured}}$. B) Plot of the force imbalance for an equi-biaxial stretch as a function of the ratio of the specimen width to the rake length ratios ($l_0/l_r$) for a range of applied strains $\alpha$. 

\[
\begin{align*}
\sum_{i=1}^{N} T_x^{(i)} &= T_x^{\text{measured}} \\
\sum_{i=1}^{N} T_y^{(i)} &= T_y^{\text{measured}} 
\end{align*}
\]
current study are also applicable to rake-suture anchored samples, and do not represent accurate predictions. Similar to rigidly clamped cruciform samples, a rigorous inverse FE analysis of rake anchored biaxial tests should be performed to accurately relate measured force to material stress.
Bibliography


Chapter 5

Compressibility of Arterial Tissue and Consequences for Modelling Soft Tissues

Abstract

Arterial tissue is commonly assumed to be incompressible. While this assumption is convenient for both experimentalists and theorists, the compressibility of arterial tissue has not been rigorously investigated. In the current study we present an experimental-computational methodology to determine the compressibility of aortic tissue and we demonstrate that specimens excised from an ovine descending aorta are significantly compressible. Specimens are stretched in the radial direction in order to fully characterise the mechanical behaviour of the tissue ground matrix. Additionally biaxial testing is performed to fully characterise the anisotropic contribution of reinforcing fibres. Due to the complexity of the experimental tests, which entail non-uniform finite deformation of a non-linear anisotropic material, it is necessary to implement an inverse finite element (FE) analysis scheme to characterise
the mechanical behaviour of the arterial tissue. Results reveal that ovine aortic tissue is highly compressible; an effective Poisson’s ratio of 0.44 is determined for the ground matrix component of the tissue. It is also demonstrated that correct characterisation of material compressibility has important implications for the calibration of anisotropic fibre properties using biaxial tests. Finally it is demonstrated that correct treatment of material compressibility has significant implications for the accurate prediction of the stress state in an artery under in vivo type loading.

5.1 Introduction

Biological soft tissues are commonly assumed to be incompressible, such that material volume is conserved under all loading configurations and only isochoric deformation occurs (Holzapfel, 2000). This assumption has important consequences for the interpretation of experimental data and for the formulation of constitutive laws. Conservation of volume imposes the kinematic constraint that the determinant of the deformation gradient $F$ must always equal unity. This lemma simplifies analysis of mechanical tests on tissues. For instance in interpreting biaxial stretching in the 1- and 2-directions the out-of-plane component of the deformation gradient of an incompressible material is trivially given as $F_{33} = 1/(F_{11}F_{22})$. The deformation gradient can then be used to calculate the Cauchy stress from the experimentally measured nominal/first Piola–Kirchhoff stress.

The incompressibility assumption also simplifies theoretical analysis of soft tissue, allowing for the formulation of constitutive laws based only on isochoric invariants and reducing the required number of material parameters (Humphrey et al., 1987; Sacks, 2000). Several soft tissues exhibit anisotropy due to the preferential alignment of collagen or elastin fibres (e.g. arteries (Dobrin, 1986), cartilage (Huang et al., 2005), annulus fibrosis (Elliott and Setton, 2001), tendons (Vilarta and Vidal,
A common approach to the modelling of fibre reinforced anisotropic soft tissue is to assume incompressibility, and hence formulate the contributions of the isotropic matrix and fibres in terms of isochoric invariants (Holzapfel et al., 2000; Holzapfel and Ogden, 2008; Humphrey et al., 1987; Sacks, 2000). Enforcement of material incompressibility (e.g. via a penalty method or a Lagrange multiplier used in conjunction with mixed/hybrid finite element formulations) is required in finite element implementations of such laws.

Despite the widespread assumption of material incompressibility, supporting experimental evidence has not yet been established for many types of soft tissue. In fact, several experimental studies suggest that cartilage is compressible (Peña et al., 2007; Smith et al., 2001). Based on such experimental observations several authors have treated soft tissue as compressible, but incorrectly used isochoric based hyperelastic models. A recent study by Nolan et al. (2014) highlights the significant errors and unphysical results that emerge when perfect material incompressibility is not enforced in an anisotropic hyperelastic formulation that is constructed using isochoric invariants.

Arterial tissue is probably the most widely studied soft tissue, both experimentally and computationally. Computational models of arteries generally assume incompressibility, with the experimental study of Carew et al. (1968) frequently cited as support for this assumption. However, Carew et al. in fact report volume changes of arterial tissue due to lumen inflation and conclude that the material is slightly compressible, but may be regarded as incompressible at small strains. Other studies (performed three to six decades ago)suggest that arterial tissue may be considered to be slightly compressible (Chuong and Fung, 1984; Lawton, 1954; Tickner and Sacks, 1967). Recent reviews of the literature (Di Puccio et al., 2012; Yosibash et al., 2014) have critiqued techniques previously used to measure arterial compressibility and concluded that a contemporary study of the topic is warranted.
The current study presents a methodology to assess the compressibility of arterial tissue and parse the isotropic ground matrix and anisotropic fibre contributions. Cylindrical discs of ovine arterial tissue are stretched in tension in the radial material axis. The volume of the specimen is measured before and after stretch using an imaging technique. Additionally, confined compression experiments are performed in order to demonstrate material compressibility under a compressive loading mode. Next, a calibration of material constants for a compressible anisotropic hyperelastic constitutive law is performed using biaxial experimental test data. Finally, the influence of compressibility on predictions of arterial compliance and wall stress is examined through the finite element simulation of artery inflation under an increasing lumen pressure.

5.2 Materials and Methods

5.2.1 Compressible Anisotropic Constitutive Model

The incompressible anisotropic hyperelastic constitutive model for collagen fibre reinforced soft tissues by Holzapfel et al. (2000) (HGO model) is commonly used to simulate arterial tissue. In a recent paper Nolan et al. (2014) demonstrate that significant errors and unphysical behaviour are computed if the incompressibility requirement is not correctly enforced for this formulation. To overcome this limitation Nolan et al. (2014) present a modified anisotropic (MA) model, a modification of the HGO model for simulation of compressible soft tissue. Based on the HGO model, the strain energy potential is additively decomposed into isotropic and anisotropic parts reflecting the anatomical structure of soft tissues ($\Psi = \Psi_{\text{iso}} + \Psi_{\text{aniso}}$). The isotropic term is a neo-Hookean material representative of the ground matrix of the tissue, while the anisotropic term represents the reinforcing collagen fibres embedded in the ground matrix. Importantly, in the MA model total anisotropic
invariants \((I_i)\), rather than isochoric anisotropic invariants \((\bar{I}_i)\), are used to describe fibre stretching so that both isochoric and volumetric deformations contribute to the anisotropic stress tensor. The anisotropic strain energy is given as

\[
\Psi_{\text{aniso}} = \frac{k_1}{k_2} \sum_{i=4,6} \exp \left\{ [k_2(I_i - 1)^2] - 1 \right\}.
\]

The total Cauchy stress for the MA model is,

\[
\sigma = \kappa (J - 1) \mathbf{I} + \frac{\mu}{J^{5/3}} (\mathbf{b} - \frac{1}{3} I_1 \mathbf{I})
+ \frac{2k_1}{J} \sum_{i=4,6} (I_i - 1) \exp \left[ k_2(I_i - 1)^2 \right] \mathbf{a}_i \otimes \mathbf{a}_i,
\]  

(5.1)

where the first term on the right hand side represents the hydrostatic stress contribution due to volumetric deformation of the compressible ground matrix, the second term represents the deviatoric stress contribution due to isochoric deformation of the ground matrix, the third term represents the total (both hydrostatic and deviatoric) anisotropic fibre stress contribution. \(J\) is the determinant of the deformation gradient \(\mathbf{F}\), \(\mathbf{b} = \mathbf{FF}^T\) is the left Cauchy-Green deformation tensor and \(\mathbf{C} = \mathbf{F}^T \mathbf{F}\) is the right Cauchy-Green deformation tensor. The first invariant \(I_1\) is the trace of \(\mathbf{b}\), \(\mathbf{I}\) is the identity tensor, \(I_i\) \((i = 4, 6\) when two fibre families are present) is the anisotropic invariant defined as \(I_i = \mathbf{a}_{0i} \cdot (\mathbf{Ca}_{0i})\) where \(\mathbf{a}_{0i}\) is a unit vector indicating the direction of fibre reinforcement and \(\mathbf{a}_i\) is the same vector in the deformed configuration given by \(\mathbf{a}_i = \mathbf{Fa}_{0i}\), \(k_1\) and \(k_2\) are material constants. The operator \(\otimes\) is the dyadic product of vectors and results in a second order tensor.

If we assume that there are two families \((i = 4, 6)\) of symmetric reinforcing fibres that are confined to the \(\theta - z\) plane (Holzapfel et al., 2000) then the unit vector \(\mathbf{a}_{0i}\) may be defined be a single parameter, an angle \(\beta\) (see Figure 5.2B) where \(\mathbf{a}_{04} = \begin{bmatrix} \cos(\beta) & \sin(\beta) & 0 \end{bmatrix}^T\) and \(\mathbf{a}_{06} = \begin{bmatrix} \cos(\beta) & -\sin(\beta) & 0 \end{bmatrix}^T\). In this case five material constants are required for the complete calibration of Equation (5.1): two isotropic constants \(\mu\) and \(\kappa\), and three anisotropic constants \(k_1\), \(k_2\) and the fibre
angle $\beta$.

5.2.2 Compressibility of Arterial Tissue

5.2.2.1 Tissue Preparation

The descending aorta is excised from six sheep sourced from a local abattoir (Brady’s, Athenry, Ireland). The vessels are stored at $-80^\circ$C until required, at which point they are defrosted in phosphate buffer solution at $3^\circ$C. Any excess connective tissue is carefully removed from the surface of the tunica externa with a scissors and scalpel. The vessel is cut along its axis as shown in Figure 5.1A and opened into a planar sheet. A circular punch with a diameter of 10 mm is used to cut out cylindrical disc specimens from this planar sheet for testing. The thickness of each specimen is measured with a micrometer. A total of 13 specimens are excised and tested.

5.2.2.2 Tensile Tests

Specimens are affixed between two platens using a cyanoacrylate adhesive (Loctite, Dusseldorf, Germany) (Figure 5.1B). This assembly is then installed into a uniaxial mechanical testing machine (Zwick Z2.5, Ulm, Germany). The crosshead position of the machine is adjusted to ensure that the specimens are in a load free configuration at the start of the test. The specimens are then subjected to a tensile nominal stretch ratio $\lambda_{\text{nom}} = 1.28$ (where $\lambda_{\text{nom}} = (b - a)/(b_0 - a_0)$, see Figure 1B) and then returned to their original state. This procedure is performed for two cycles. Force is recorded throughout the experiment and identical force–displacement curves for the two cycles indicate that the specimen has not been damaged, nor has it detached from the platen during the test. A camera system (1.31 MPx, 25 fps; uEye, IDS, Obersulm, Germany; videoXtens software, Zwick, Ulm, Germany) is set up to record the in-plane deformation of the cylindrical specimen as it is stretched. Images of the specimen are analysed in the initial state, and when fully stretched. These images
Figure 5.1: **A)** Schematic outlining the specimen extraction. Tubular sections of arterial tissue from the descending aorta are cut along their axis to form planar sheets. A circular punch is used to cut cylindrical specimens from the planar sheet. **B)** Schematic and images of the experiments performed to determine the compressibility of arterial tissue. Discs of arterial tissue are secured between two platens and an initial image is taken to determine $V_i$ the initial volume of the disc. The artery is subsequently stretched and a further image is taken to determine the stretched volume $V_s$ along with the force measured by the load-cell at this stretch. **C)** Flowchart outlining the inverse FE method used to determine the isotropic (ground matrix) material properties of arterial tissue. Assuming a neo–Hookean hyperelastic material, one may iteratively solve for the bulk modulus $\kappa$ and shear modulus $\mu$ of the ground matrix. An axi-symmetric FE simulation of the above experiment is performed and the resultant force and volume change are computed and compared to the experimentally measured values. The values of $\kappa$ and $\mu$ are iterated upon until a satisfactory match between the computational and experimental data is achieved. **D)** Schematic outlining a confined compression experiment on cylindrical specimens of arterial tissue (identical to those in A)). A load is applied using a cylindrical indenter, specimens are not permitted to deform in the lateral direction. Confined compression results are used to validate $\mu$ and $\kappa$ (determined in Figure 1C).
are then used to compute volume change of the specimen during the test.

5.2.2.3 Volume Change Measurement

Images of the geometric profile of specimens are outlined using ImageJ (Schneider et al., 2012) image processing software. The profiles are exported as a set of coordinates for 40 points on the free surface of the specimen. The radius of the specimen $y(x)$ is calculated at each of these 40 points (see Figure 5.1B). To compute the specimen’s volume the trapezoidal rule is used to evaluate the following integral:

$$V = \pi \int_{a}^{b} y(x)^2 \, dx,$$

(5.2)

where $a$ is the $x$-position of the fixed platen and $b$ is the $x$-position of the moving platen. Using this method, the initial specimen volume $V_i$ and deformed specimen volume $V_s$ are calculated. A second quasi-3D methodology for estimation of the volume change using two two orthogonal camera projections of the deformed samples is presented in Appendix C. No statistically significant difference is calculated between the two methodologies of computing the sample volume change. The ratio of the volume change is given by $\Delta V/V_i = (V_s - V_i)/V_i$. If the tissue were truly incompressible then no volume change would be observed during the test. On the other hand, an observed volume change means that the material is compressible.

5.2.2.4 Calibration of Isotropic Ground Matrix

To further quantify the compressibility of arterial tissue, the above experiments are simulated using FE analysis. The MA model for compressible fibre reinforced soft tissue is presented in Section 5.2.1. It is generally assumed that fibres do not contribute to stress in compression (i.e. if $I_i < 1$ then $\Psi_{\text{aniso}} = 0$). In the above experiment, the specimen is stretched in the material’s radial direction, causing a
lateral contraction in the $\theta - z$ plane. Therefore a fibre contribution is not expected in this mode of applied loading. Rather, it is expected that the material stress and deformation is governed by the isotropic ground matrix, i.e. the first two terms of the right hand side of Equation 5.1, characterised by the bulk modulus $\kappa$ and the shear modulus $\mu$. Even though the isotropic ground matrix is described by a hyperelastic material model, an effective material Poisson’s ratio $\nu_{\text{eff}}$ can be determined from the calibrated values of $\kappa$ and $\mu$, given in Equation 5.3 as

$$\nu_{\text{eff}} = \frac{3\kappa/\mu - 2}{6\kappa/\mu + 2}. \quad (5.3)$$

Initial simulations are performed to established that the anisotropic fibre terms do not contribute to the material stress and deformation under the applied loading mode. Next, an inverse FE scheme is employed to calibrate $\kappa$ and $\mu$ from the experimental data, as outlined in Figure 5.1C. Briefly, trial bulk and shear moduli are set and an axisymmetric FE simulation of the experiment is performed. From this the resultant stretching force in the vertical direction (i.e. the force the load cell experiences) and the percentage change in volume are computed. The bulk and shear moduli are iterated upon until the experimentally measured stretching force and volume change are achieved.

All FE simulations are performed using Abaqus/Standard (v6.13-2, DS Simulia, RI, USA). Equation (5.1) is implemented in Abaqus via a user-defined Fortran subroutine (UMAT), for details of the consistent tangent matrix refer to Nolan et al. (2014). The artery geometry in the undeformed reference configuration is constructed from experimental images taken before the load application (mean specimens geometric parameters for a range of tested samples, $n=10$). A mesh sensitivity study reveals that a mesh consisting of 3,000 four noded axisymmetric elements provides a converged solution. Mirroring the experimental set-up, the bottom face of
the cylinder is fully constrained in the $r$, $\theta$ and $z$ directions while the top face of the cylinder is displaced in the $z$ direction to a nominal stretch of 1.28 whilst constrained in the $r$ and $\theta$ directions.

5.2.2.5 Confined Compression Tests

To further assess the compressibility of arterial tissue and validate the material parameters calculated for the ground matrix, a series of confined compression tests were performed on cylindrical specimens of arterial tissue ($n = 9$). Figure 5.1D outlines a schematic of the experiment. A specimen is placed into a rigid die, thus preventing any lateral deformation. Specimens are deformed by a cylindrical punch; axial nominal strains of 10% are applied. The experimental confined compression axial stress-strain relationship is then compared to predicted theoretical response using the compressible material properties determined from the tension tests described in Section 5.2.2.4.

5.2.3 Biaxial Experiments

Biaxial stretch tests using cruciform specimens of arterial tissue are performed. An inverse FE method is used to interpret the biaxial tests and calibrate the constitutive model in Equation 5.1.

5.2.3.1 Specimen Preparation

Specimens are excised from five ovine descending aortas using a custom made cruciform template. The geometry of the cruciforms are outlined in Figure 5.2B. Cruciform arms are aligned with the axial and circumferential directions of the artery. Specimens have a half width $w_0 = 4$ mm, a half length $l_0 = 12$ mm, and a fillet radius $R = 3$ mm. The thickness of each specimen is measured using a micrometer.
Chapter 5

Figure 5.2:  A) Schematic of the biaxial experiment. A cruciform shaped tissue specimen is held rigidly in clamps. Each clamp is rigidly fixed to a load cell which in turn is rigidly fixed to a linear actuator controlling the displacement of the clamp. Force–displacement data are acquired in the $x$ and $y$ axes. Two displacement ratios, $u_x/u_y = 1$ and $u_x/u_y = 2$ are examined in the current study. B) Schematic indicating the boundary conditions of the biaxial experiment outlined above in A. In this setup, displacements are imposed at each of the clamps ($u_x$ and $u_y$) and the resultant forces ($F_x$ and $F_y$) are measured. The two families of reinforcing fibres are indicated at angles $\pm \beta$. 

---

A

B

Clamp $y$

Clamp $x$

Tissue specimen

Load cell

Linear actuator

$T_{x, u_x}$

$T_{y, u_y}$

$R$

$w$

$l_o$

$\beta$

$\beta$

$x$

$y$
Chapter 5

A total of four specimens are tested.

5.2.3.2 Biaxial Test Protocol

Figure 5.2A shows a schematic of the biaxial experimental set-up. The test apparatus consists of four fixed linear actuators which may be independently controlled. Each actuator houses a 100 N load cell which in turn is connected to the jaws. The jaws themselves have a roughened surface to prevent slippage during testing. Specimens are loaded into jaws with the circumferential direction $\theta$ aligned with the $x$-axis and the axial direction $z$ with the $y$-axis of the machine (see Figure 5.2B). Biaxial tests are performed on each of the specimens ($n = 6$) at a clamp displacement rate of 0.025 mm/s. Specimens are tested using two different clamp displacement ratios, $u_x/u_y = 1$ and $u_x/u_y = 2$. The testing protocol is briefly outlined as follows. An equi-biaxial stretch ($u_x/u_y = 1$) to a maximum clamp displacement of 3 mm is first performed. The clamps are returned to their original position and a rest period of 120 s is allowed before an non-equi-biaxial test ($u_x/u_y = 2$) is performed where $u_{x\text{ max}} = 3$ mm. For each specimen, this procedure is repeated five times.

5.2.3.3 Inverse FE Analysis for Calibration of Anisotropic Fibres

Data collected from biaxial tests together with the shear and bulk modulus of the matrix (determined using the methodology described in Section 5.2.2) are used to calibrate the model parameters in the anisotropic terms of Equation (5.1). The biaxial tests yield four independent sets of force-displacement data, one for each material axis for a given clamp displacement ratio. For a complete calibration, each material constant requires an independent data set. In the case of the MA constitutive model three material constants must be calibrated, $k_1$, $k_2$, $\beta$. The biaxial tests provide sufficient data for calibration and an additional data set for verification. The relationship between the experimentally measured force and the
Chapter 5

Figure 5.3: Flowchart outlining the iterative inverse FE method used to determine material properties. An initial guess of the material properties is made for the first iteration \((n = 1)\). Using this set of parameters, the objective function is evaluated. This is a two step process, firstly for each displacement ratio examined, an equivalent FE simulation is performed using the parameters defined in \(\Lambda^{(n)}\). The net force–displacement \((F–u)\) curves at each of the clamps are computed. Secondly, the FE computed force–displacement curves at each clamp for each displacement ratio are compared to their experimental counterpart using a least-squares regression method. The objective function is calculated by summing the \(r^2\) values for each of the performed regressions. Here \(ntests\) is the number of displacement ratios examined and in this case is 2, \(naxes\) are the number of clamp force–displacement data sets and in this case is also 2 (x and y clamps). The objective function is then checked for convergence by comparing it to a tolerance set by the user. If the optimization has converged then the process is terminated. If it has not converged, the value of \(f(\Lambda^{(n)})\) is returned to the optimization algorithm and a new set of material parameters \(\Lambda^{(n+1)}\) is created. The process is then repeated; the objective function is evaluated and checked for convergence with new material parameters being set each time until convergence is achieved.

\[
\Lambda^{(n)} = \{k^{(n)}, k_2^{(n)}, \beta^{(n)}\}; \quad n = 1
\]

\[
f(\Lambda^{(n)}) = \sum_{i=1}^{ntests} \sum_{j=1}^{naxes} (1 - r^2)
\]

\[
\text{Clamp } y; \quad u_1/u_2 = 1
\]

\[
T \quad \text{FE} \quad \text{Exp}
\]

\[
r^2 = 0.86
\]
material stress in a biaxial test is complex. Recently Nolan and McGarry (2015) demonstrated that the stress distribution in a cruciform specimen subjected to a biaxial stretch is highly non-uniform and cannot be trivially related to the measured force. Therefore an inverse FE scheme based on the force-displacement experimental data must be employed to accurately characterise the material behaviour.

Figure 5.3 shows a flowchart describing the inverse FE method. This entails an optimization/minimization problem where a trial set of parameters $\Lambda$ are initially created and evaluated by an objective function $f(\Lambda)$. If $f(\Lambda)$ meets the convergence criteria then the process is terminated, if not then a new set of parameters are created by the optimization algorithm and the process is repeated. Specifically the set of parameters we wish to determine are the anisotropic material constants for the compressible MA constitutive model from Equation 5.1; i.e. $\Lambda = \{k_1, k_2, \beta\}$. The objective function consists of two parts. The first part are the force-displacement curves established from the FE simulation of the biaxial tests, which replicate the geometry and boundary conditions of the experiments. Simulations are performed for the displacement ratios $u_x/u_y = 1$ and $u_x/u_y = 2$. For each simulation, net force-displacement curves at the $x$ and $y$ clamps are computed. The second part quantifies how closely the FE simulation reproduces the experimental data. A least-squares regression is calculated comparing the experimental and FE force-displacement curves. The correlation coefficient $r^2$ is computed for the four sets of force-displacement data. As the correlation improves $r^2 \to 1$; $(1 - r^2)$ quantifies the goodness of fit. The objective function then is the sum of the goodness of fit measures, for the $n^{th}$ iteration,

$$f(\Lambda^{(n)}) = \sum_{1}^{n_{ratio}} \sum_{1}^{n_{axes}} (1 - r^2),$$  

(5.4)

where $n_{ratio}$ are the number of unique displacement ratios used in the biaxial testing
Figure 5.4: Barchart indicating the percentage volume change measured in each of the specimens tested. The mean value for the volume change \((\pm S.D.)\) is 9.31±3.19%. All specimens exhibit volume change and hence should be regarded as compressible.

and \(\text{naxes}\) are the number of axes the material is tested in. In the current study \(\text{nratio} = 2\) and \(\text{naxes} = 2\). Convergence is judged to have occurred when the change in \(f(\Lambda)\) is less than a predefined tolerance value. If convergence does not occur, a derivative-free, Nelder-Mead simplex algorithm (Nelder and Mead, 1965; Lagarias et al., 1998) is used to determine the next parameter set \(\Lambda^{(n+1)}\) that should be evaluated by the objective function.

### 5.3 Results

#### 5.3.1 Compressibility of Arterial Tissue and Isotropic Ground Matrix Calibration

To assess whether any specimen damage, debonding, or plasticity occurs during the test protocol described in Section 5.2.2.2, successive loading cycles are analysed. In all cases the measured force-deformation curves are identical for successive cycles, indicating that only elastic deformation of the specimens occurs, as expected, with the bond between the specimen and the loading platens remaining fully intact.
throughout (also confirmed by post-test examination). The measured force when the specimen is fully stretched (±S.D.) is 0.59 ± 0.21 N (n = 13). Using the method outlined in Section 5.2.2.3 the specimen volume change following load application is determined. Figure 5.4 shows a bar chart of the percentage volume change in each of the specimens tested (n = 13); the mean percentage volume change (±S.D) is 9.31 ± 3.19%. Note that a volume change is determined in all cases, demonstrating that the assumption of material incompressibility is not appropriate for arterial tissue.

Finite element simulations confirm that fibres shorten under the applied mode of loading, so that experimental data can provide an independent calibration of the isotropic matrix parameters $\kappa$ and $\mu$. An inverse FE study is performed to determine the parameter values that result in the experimentally observed percentage volume change of 9.31% for an applied force of 0.59 N. Results are shown in Table 5.1. For completeness, calibrations are also performed using target experimental values one standard deviation above and below the mean values, providing upper and lower limits for the material constants. As reported in Table 5.1, using (5.3), the effective Poisson’s ratio of the arterial tissue ranges from 0.412 to 0.469, again indicating that the material is indeed compressible.

5.3.2 Confined Compression Test Results

Figure 5.5 shows the experimental axial stress-strain curve for the confined compression test (mean±S.D.). Also shown is the predicted stress-strain curve using the compressible neo–Hookean material parameters determined from the tension tests in Section 5.3.1 (mean, upper and lower bounds given in Table 5.1). The experimental and predicted confined compression data are in good agreement with one another. This result provides a validation of the material parameters for the compressible ground matrix determined in Section 5.3.1 above. It should be noted that the axial
<table>
<thead>
<tr>
<th></th>
<th>$\Delta V/V_0$ (%)</th>
<th>$\mu$ (kPa)</th>
<th>$\kappa$ (kPa)</th>
<th>$\kappa/\mu$</th>
<th>$\nu_{eff}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Upper</td>
<td>12.50</td>
<td>7.87</td>
<td>42.14</td>
<td>5.34</td>
<td>0.412</td>
</tr>
<tr>
<td>Mean</td>
<td>9.31</td>
<td>6.47</td>
<td>56.66</td>
<td>8.56</td>
<td>0.445</td>
</tr>
<tr>
<td>Lower</td>
<td>6.12</td>
<td>6.25</td>
<td>99.03</td>
<td>15.79</td>
<td>0.469</td>
</tr>
</tbody>
</table>

Table 5.1: Table of the material properties $\kappa$ and $\mu$ computed from the inverse FE scheme outlined in Figure 5.1C using the mean value of force measured in the experiments and $\pm$ one standard deviation as the upper and lower bounds.

Figure 5.5: Stress-strain curve for confined compression tests ($n = 9$). Also shown is the predicted stress-strain behaviour, based on a neo-Hookean constitutive law and the compressible material parameters determined from the tensile tests (Table 5.1). Note that the axial strain $\varepsilon_{xx}^{nom}$ is equal to the volumetric strain $\Delta V/V_0$ in confined compression.
Figure 5.6: Calibration of the biaxial tests using the compressible MA model. Force-displacement curves for clamps $x$ and $y$ and displacement ratios $u_x/u_y = 1$ and $u_x/u_y = 2$. The solid lines are the experimentally measured curves whilst the symbols represent the best fit FE solution. The cost function for this calibration is $f(\Lambda) = 0.072$ while the lowest value of the correlation coefficient $r^2 = 0.97$. Material parameters are give in Table 5.2.

strain $\varepsilon_{xx}^{\text{nom}}$ is equal to the volumetric strain $\Delta V/V_0$ in this confined compression experiment.

5.3.3 Anisotropic Material Constant Calibration

The anisotropic material properties $k_1$, $k_2$ and $\beta$ for the MA constitutive model given in Equation (5.1) are determined from biaxial tension experiments using the method outlined in Section 5.2.3.3. The mean force-displacement curve ($n = 6$) is used as the target experimental data and a mean specimen thickness of 2.9 mm is assigned to the FE model. Table 5.2 gives the material properties determined from this analysis and Figure 5.6 plots normalized force–displacement curves in the $x$ and $y$ directions for biaxial displacement ratios of $u_x/u_y = 1$ and $u_x/u_y = 2$. A good correlation between the measured experimental data and calibrated FE simulations is achieved ($r^2 > 0.97$ for all plots). As expected, highly anisotropic material behaviour is
### Table 5.2: Results from the inverse FE scheme for the anisotropic material parameters of the MA model defined in Equation 5.1.

<table>
<thead>
<tr>
<th>$k_1$ (kPa)</th>
<th>$k_2$</th>
<th>$\beta$ (°)</th>
<th>$r^2$</th>
<th>$f(\Lambda)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.81</td>
<td>1.98</td>
<td>60.2</td>
<td>0.97</td>
<td>0.07</td>
</tr>
</tbody>
</table>

Figure 5.7: Calibration of the biaxial tests using the incompressible HGO model. Mean force-displacement curves for clamps $x$ and $y$ and displacement ratios $u_x/u_y = 1$ and $u_x/u_y = 2$. The solid lines are the experimentally measured curves whilst the symbols represent the best fit FE solution. The cost function for this calibration is $f(\Lambda) = 0.071$ while the lowest value of the correlation coefficient $r^2 = 0.97$.

observed, with the measured force being significantly higher in the circumferential direction of the sample. It should also be noted that force–displacement curves are quite linear, with no significant strain stiffening being observed over the range of applied deformation (the maximum principal nominal strain at the centre of the specimen $\varepsilon_{\text{nom}}^{\text{max}} = 25\%$ at maximum extension).

Additionally in Appendix B we perform specimen-specific calibrations of each biaxial test, where unique specimen thickness' and force-displacement curves are used.
5.3.4 Assessment of Error Generated by the Incompressibility Assumption

Having established in Section 5.3.1 that aorta arterial tissue is compressible, we next assess the errors introduced by the commonly used assumption of material incompressibility. Assuming that the material is incompressible, a ground matrix shear modulus is calibrated using the method outlined in Section 5.2.2.4. The experimentally measured volume change is neglected, and the inverse FE method is matched using just the force data. A shear modulus of $\hat{\mu} = 5.2$ kPa (where the hat symbol, $\hat{}$, indicates the material parameter is for the incompressible HGO model) is found to reproduce the experimentally measured mean applied force of 0.59 N at $\lambda_{\text{nom}} = 1.28$ nominal stretch ratio (see Figure 5.1), but with no volume change permitted. Next the anisotropic material parameters for the incompressible HGO model (Holzapfel et al., 2000) are calibrated from the biaxial test data using the inverse FE procedure outlined in Section 5.2.3.3. Anisotropic material constants of $\hat{k}_1 = 6.92$ kPa, $\hat{k}_2 = 0.89$ and $\hat{\beta} = 57.5^\circ$ are determined (see Figure 5.7). In Figure 5.7 it appears that a very accurate calibration of the material properties has been achieved using the incompressible HGO model ($r^2 > 0.97$). However, noting that this calibration has been performed while ignoring the material compressibility determined in Section 5.3.1, we next demonstrate that significant errors may be encountered by the inaccurate incompressibility assumption in a tri-axial loading environment. Specifically we consider the case of an artery expansion under increasing lumen pressure using both the compressible MA model and the incompressible HGO model. The artery is modelled as a three-dimensional thick walled cylinder with fixed ends (no net out-of-plane deformation is permitted in the $z$-direction). Figure 5.8A illustrates the geometry and boundary conditions in addition to the applied lumen pressure $L_P$. The artery is inflated up to a maximum lumen pressure ($L_{P_{\text{max}}}$) of 4.0 kPa. A mesh sensitivity study determines that 1,600 elements result in a sufficiently converged
Figure 5.8:  A) Schematic of a quarter artery showing the geometry and required boundary conditions used for the FE simulations. The artery has an internal radius \( r_i = 9 \text{ mm} \) and an external radius \( r_e = 12 \text{ mm} \) and is subjected to an internal lumen pressure \( L \text{P}_{\text{max}} = 4.0 \text{ kPa} \). B) Plot showing the predicted internal and external radial strain (\( \Delta r/r_0 \)) with increasing lumen pressure \( L \text{P} \) for the compressible MA model and the incompressible HGO model. C) Contour plot of the axial Cauchy stress \( \sigma_{zz} \) over the circumferential Cauchy stress \( \sigma_{\theta\theta} \) (the plane in which the reinforcing fibres are located) computed by the HGO and MA models. The contour shows a marked difference in the stress distribution in the artery wall. D) Contour plot of the stress triaxiality \( p/q \) in the artery wall computed by the HGO and MA model. Stress triaxiality is the pressure stress \( p \) over the von Mises stress \( q \). Again we see marked differences in the triaxiality of the stress. Note that all contour plots are plotted in the undeformed configuration for the purposes of comparison.
solution. We ensure that the maximum principal strain in the vessel wall does not exceed the maximum strain used in calibrating the models. Figure 5.8B plots the internal and external radial strain ($\Delta r/r_0$) with increasing lumen pressure ($LP$) for both the MA and HGO models. Both models predict near identical arterial compliance. This simulation is analogous to a 1:0 biaxial stretch in the $\theta - z$ plane with an additional small compressive stress in the radial direction. The $\sigma_{\theta\theta}$ and $\sigma_{zz}$ stress components are at least two orders of magnitude greater than the $\sigma_{rr}$ radial stress, highlighting that the dominant deformation occurs primarily in the plane of the fibres. Given that the MA and HGO models are calibrated to give an identical response in biaxial tension (see Figures 5.6 and 5.7 respectively), a similar arterial compliance is computed by both models as shown in Figure 5.8B.

However the calibrated MA model, which correctly accounts for compressibility, predicts a very different stress state in the artery wall to the HGO model which does not account for compressibility. Figure 5.8C-D demonstrate that the entire stress distribution is significantly affected. Figure 5.8C considers the stress biaxiality in the artery wall, i.e. the ratio of the axial to circumferential stress ($\sigma_{zz}/\sigma_{\theta\theta}$). The models compute a significantly different magnitude and gradient of stress biaxiality through the artery wall. Clearly the incompressibility assumption has significant implications for the out-of-plane axial stress ($\sigma_{zz}$) component, with important consequences for prediction of artery buckling stress (Ghriallais and Bruzzi, 2013), etc. Figure 5.8D considers the stress triaxiality in the artery wall; the ratio of the pressure stress ($p = \text{tr}(\sigma)$) to the von Mises stress ($q = \sqrt{(3/2)\sigma':\sigma'}$ where $\sigma'$ is the deviatoric stress). Stress triaxiality is an indication of the volumetric to deviatoric (shear) stress at a material point and is often used as a scalar measure of a tri-axial stress state. Additionally stress triaxiality has been shown to be an important factor in crack nucleation and material rupture (Rice and Tracey, 1969). Significant differences in stress triaxiality magnitude and gradient are computed even though both
Chapter 5

Table 5.3: Values of the von Mises stress ($q$), pressure stress ($p$), axial stress ($\sigma_{zz}$), and circumferential stress ($\sigma_{\theta\theta}$) at internal radius, $r_i$, and the external radius, $r_e$.

| $r_i$ ($q$ (kPa)) | 32.26 | 11.98 | 30.69 | 13.22 |
| $r_e$ ($p$ (kPa)) | 10.95 | 5.55  | 9.93  | 6.52  |
| $r_i$ ($\sigma_{zz}$ (kPa)) | 4.42  | 3.59  | 4.68  | 4.18  |
| $r_e$ ($\sigma_{\theta\theta}$ (kPa)) | 31.96 | 13.24 | 29.81 | 14.97 |

models have been accurately calibrated to biaxial test data ($r^2 > 0.97$) and exhibit similar material compliance. The values of $q$, $p$, $\sigma_{zz}$, and $\sigma_{\theta\theta}$ at the internal and external radius for both the HGO and MA models are given in Table 5.3. Taking the compressible model as giving the correct predictions of stress, the error in the stress triaxiality is 7% and the error in the stress biaxiality is 3%, at the external radius of the artery.

Appendix D simulates lumen inflation where residual stresses in the vessel wall have been included. Results show that, once again, compressibility of the tissue has an important influence on the stress-state in the vessel wall.

5.4 Discussion

The current study provides new insight into the compressibility of arterial tissue. The key findings of the study are as follows:

1. Aortic arterial tissue is compressible. Stretching of aortic tissue specimens in the radial direction reveals significant volume changes (mean $\Delta V/V_0 = 9.31\%$).

2. Biaxial stretch experiments alone are not sufficient to characterise tissue behaviour. We demonstrate that the incompressible HGO model and its modified compressible form (MA model) can both be accurately calibrated to capture experimental biaxial test data ($r^2 > 0.97$ for both), despite the fact the HGO
model neglects material compressibility.

3. Failure to accurately characterize tissue compressibility will result in the inaccurate prediction of artery wall material stress in vivo, even if artery compliance is accurately calibrated.

Previously published material models assume that arterial tissue is incompressible (Chuong and Fung, 1983; Gasser et al., 2006; Holzapfel et al., 2000; Sun and Sacks, 2005), as do many experimental studies (Hayashi et al., 1980; Humphrey et al., 1987; Raghavan and Vorp, 2000; Sacks, 2000; Takamizawa and Hayashi, 1987). The paper by Carew et al. (1968) is generally cited as justification for the assumption of incompressibility. Carew et al. (1968) expanded segments of artery under physiological lumen pressure and the change in volume of the artery tissue was measured. No significant volume change was observed but critically the study is limited to the small strain regime. Moreover the study of DiPuccio et al. (Di Puccio et al., 2012) suggests that accuracy of the technique used by Carew et al. should be improved upon. Previous studies have attempted to measure volume change by directly measuring artery geometry (Boutouyrie et al., 2001; Dobrin and Rovick, 1967). During lumen expansion the change in vessel thickness scales with the square root of the volume change. Hence in a lumen expansion experiment, the measurement of volume change via the change in internal and external radii requires very accurate measurement and presents a considerable experimental challenge.

In the current study a novel combined experimental and computational approach is developed to overcome this challenge. By stretching aortic arterial tissue in the radial direction and monitoring resultant changes in the tissue volume, it is shown that aortic ground matrix material exhibits significant compressibility. This methodology for the determination of tissue compressibility is based on experimental evidence that fibres are primarily confined to the θ – z plane (Finlay et al., 1995) and hence
do not contribute to stretching in the radial direction. A number of papers report dispersion of the fibre orientation angles in arteries (Canham et al., 1989; Finlay et al., 1998). This may lead to a small contribution of fibres in the radial direction but it is expected that this is a secondary effect as it is generally accepted that arteries have two families of fibres in the $\theta - z$ plane (Holzapfel et al., 2000; Silver et al., 1988). This novel technique allows the determination of material compressibility, while parsing isotropic contribution of the ground matrix. To further validate this finding, we perform additional experimental tests for a confined compression mode of deformation; confined compression results are in close agreement with our tension tests.

In addition to stretching in the radial direction, biaxial tests are performed to determine fibre mechanical properties. An inverse FE method is used to provide an optimal calibration of the fibre properties from the experimental results. In the current study we demonstrate that if material compressibility is not independently established, a unique set of anisotropic material properties cannot be determined through biaxial tests alone. To highlight this point we demonstrate that biaxial experimental test data can be accurately predicted by both the compressible MA material model ($r^2 > 0.97$) and the incompressible HGO material model ($r^2 > 0.97$). This is despite the fact that the aforementioned compressibility was rigorously established in Section 5.2.2. The parsing of the matrix contribution using the method in Section 5.2.2 and determination of fibre properties as shown in Section 5.2.3 provides a new and systematic approach to the mechanical characterisation of soft tissue.

In the current study aorta tissue exhibits slightly non-linear stress-strain behaviour in the strain range examined ($\varepsilon_{\text{nom}}^{\text{max}} = 25\%$ at the specimen centre at maximum extension). Such near-linear behaviour is similar to the uniaxial experimental results of Sokolis et al. (Sokolis et al., 2006). In contrast highly non-linear exponen-
tial strain stiffening has been observed for coronary and carotid arteries for strain ranges up to 30% (Humphrey, 2002; Silver et al., 2003). Future studies should investigate changes in material compressibility at very high levels of applied strain (both compressive and tensile).

The current study is the first to present rigorous quantification of aorta compressibility. Follow-on studies should be performed on other types of elastic arteries e.g. carotid, iliac arteries, as well as muscular arteries, e.g. femoral, cerebral arteries, in order to characterise ground matrix compressibility as a function of anatomical location. Given the similarities in anatomical composition of all elastic arteries (Humphrey, 2002), based on the current study it is not unreasonable to suggest that they will exhibit some degree of compressibility. Future studies should also consider both healthy and diseased human arterial tissue. It is possible that the level of compressibility aneurysmal tissue or atherosclerotic tissue may differ from that of healthy tissue. The recent study by Yosibash et al. (2014) reports volume changes in segments of porcine femoral and saphenous arteries under lumen pressure however precise characterisation of material compressibility has yet to be performed.

The significant errors that can result from an inappropriate incompressibility assumption are highlighted in Section 5.3.4 in the case study of a 3D artery subjected to a lumen pressure. In this case study the artery is subjected to a triaxial stress state hence exposing the significant errors that can be generated if material compressibility is not properly characterised. Though a change in volume of the artery wall is computed using the compressible MA model, because the change in artery wall thickness scales approximately with the square root of the volume change, a small change in artery wall volume (≈ 2%) results in a very small change in vessel radius.

The importance of compressibility on the biaxial and triaxial stress reported in this study is not surprising, based on theoretical analysis that demonstrates that stresses in thick walled elastic cylinders are dependent on compressibility (Misra
and Chakravarty, 1980). The importance of compressibility has also been demonstrated in cases where residual stress has been included. The theoretical relationship between residual stress and compressibility was previously noted (Volokh, 2006).

These alterations have important consequences for all manner of biomechanics and medical device simulations. Correct modelling of vessel compliance and stress are vital for the accurate simulation of many biomechanics and medical device problems. For example; the radial force required to deploy a stent, stent recoil and fatigue (Conway et al., 2012), for peripheral vessel buckling and deformation (Ghriallais and Bruzzi, 2013), and for prediction of abdominal aortic aneurysm rupture (Vorp et al., 1998).

5.5 Conclusion

In the current paper we have determined that aortic arterial tissue is compressible. A rigorous methodology for calibration of the isotropic ground matrix and anisotropic fibre contribution is presented. Finally we demonstrate that material compressibility must be accounted for in order to accurately predict the stress state of an artery wall.

Acknowledgements

The authors wish to acknowledge funding from Science Foundation Ireland under project SFI-12/IP/1723. Furthermore we acknowledge funding from the Irish Research Council and the College of Engineering and Informatics at NUI, Galway.
Figure 5A.1: Mean radial strain with increasing lumen pressure for i) the MA model (Equation (5.1)), ii) the MA_LNH model which uses a modified version of the neo-Hookean model to represent the ground matrix; this version uses a logarithmic penalty term $\ln(J)$ to prevent excessive volumetric deformations, and iii) the MA_HYF model which uses a hyperfoam model to represent the ground matrix.

5.6 Appendices

Appendix 5A: Investigation of different forms of $\Psi_{iso}$

In Section 5.2.1 the strain energy potential for the MA model is additively split into isotropic and anisotropic parts $\Psi = \Psi_{iso} + \Psi_{aniso}$. The MA model uses a common neo-Hookean strain energy potential, $\Psi_{iso} = \frac{\mu}{2}(I_1 - 3) + \frac{\kappa}{2}(J - 1)^2$. Here the use of two additional hyperelastic strain energy potentials for use as the isotropic term $\Psi_{iso}$ are investigated. Firstly a modified version of the standard neo-Hookean model which was developed for scenarios involving large compressive stresses is examined. Its strain energy potential is given as:

$$\Psi_{iso} = \frac{\mu}{2}(I_1 - 3) + \frac{\kappa}{2} \left( \frac{J^2 - 1}{2} - \ln(J) \right). \quad (5A.1)$$
In this model the volumetric term has been modified to include the function $\ln(J)$. This has the effect of penalising very large volume changes and prevents $J \to 0$.

Secondly a hyperfoam model Storåkers (1986) developed for highly compressible hyperelastic polymer foams is examined. Its strain energy function is given as:

$$
\Psi_{\text{iso}} = \sum_{i=1}^{N} \frac{2\mu_i}{\alpha_i^2} \left[ \lambda_1^{\alpha_i} + \lambda_2^{\alpha_i} + \lambda_3^{\alpha_i} - 3 + \frac{1}{\beta_i}(J^{-\alpha_i\beta_i} - 1) \right], \tag{5A.2}
$$

where $N$ is the order of the function, $\lambda_m$ ($m = 1, 2, 3$) are the principal stretches, $\alpha_i$ determines the non-linearity for each term in the function, $\beta_i$ determines the compressibility for each term in the strain energy function and is related to the Poisson’s ratio $\nu_i$ through the expression $\beta_i = \nu_i/(1 - 2\nu_i)$, and the initial bulk modulus $\kappa_0 = \sum_{i=1}^{N} 2\mu_i[(1 - 3\beta_i)/3]$.

Equation (5A.1) is added to the anisotropic potential of the MA model to form the MA\_LNH model and equation (5A.2) is added to the anisotropic potential of the MA model to form the MA\_HYF model. The simulations from Section 5.3.4 are repeated using the MA\_LNH and MA\_HYF models for the artery wall. The MA\_LNH model uses the mean bulk and shear modulus from Table 5.1 and the MA\_HYF model uses $N = 1$, $\alpha_i = 2$, $\nu_i = 0.44$, and $\mu_i = 7.04$ kPa.

The mean radial strain–pressure curves for both of these models, as well as that of the original MA model are given in Figure 5A.1. Use of the MA\_LNH model results in no difference in arterial compliance compared to the MA model. The MA\_HYF model computes a small difference in compliance. For the hyperfoam model it is recommended that the effective Poisson’s ratio does not exceed 0.45.
Table 5B.1: Anisotropic material parameters for the MA model defined in Equation 5.1 uniquely calibrated for each individual specimen, as well as the individual specimen thickness.

Appendix 5B: Calibration of Anisotropic Constitutive Models

Calibrations are performed for each of the six individual specimens tested using their unique force-displacement curve and the specimen thickness measured using the technique outlined in Section 5.2.3.3. The results of these individual calibrations are presented in Table 5B.1.

Appendix 5C: Quasi-3D Method for Volume Change Measurement

Volume change is calculated using an alternative method by measuring two orthogonal axes/diameters of the specimen at each segmentation plane. The volume is computed by integrating the resultant cross-sectional areas over the height of the specimen using a trapezoidal type method. A schematic outlining this method is given in Figure 5C.1. This alternative methodology results in a volume change of 10.11±4.61% (mean±S.D.). A t-test indicates that there is no statistically significant difference between the mean volume change calculated using the axi-symmetric
Figure 5C.1.: Quasi-3D calculation to determine the volume change in cylindrical specimens. Orthogonal experimental images measure the orthogonal diameters, $2a$ and $2b$, of the specimen at each segmentation plane. The volume, $V$, is calculated by integrating cross-sectional areas over the height of the specimen.

or the quasi-3D method.

**Appendix 5D: Inclusion of residual stress**

The influence of residual stresses on the stress-state in the vessel wall is assessed in this appendix. It is well established that residual stresses are present in the unpressurised vessel wall. Simulations of lumen inflation were performed, following the computational method outlined by Raghavan et al. (2004) and using the experimental data of Vaishnav and Vossoughi (1987) to determine stress-free geometry. The vessel has a stress-free internal radius $R_i = 21.92$ mm, an external radius $R_e = 24.94$ mm, and an opening angle of $80.22^\circ$. The material parameters for both the HGO and MA models are identical to those used in Section 5.3.4.

Figure 5D.1. shows a contour plot of the residual von Mises stress in the vessel wall in the unpressurised configuration. The vessel moves from a state of compression...
Figure 5D.1.: Residual (von Mises) stress in the vessel wall under zero lumen pressure for A) the incompressible HGO model, and B) the compressible MA model.

on the inner face to tension on the external face. As the anisotropic component of both the HGO and MA models are inactive in compression, this explains the higher stress on the external face of the vessel. Figure 5D.2. shows a contour plot of the ratio of the axial stress to the circumferential stress \((\sigma_{zz}/\sigma_{\theta\theta})\) for the HGO and MA models. This figure further illustrates the dependence of the stress-state on the treatment of compressibility. Differences between the HGO and MA models are similar to those shown in Figure 5.8 without residual stress. This illustrates that the important influence of compressibility on triaxial artery stress is significant regardless of the inclusion of residual stress.
Figure 5D.2.: Ratio of the axial stress to the circumferential stress ($\sigma_{zz}/\sigma_{\theta\theta}$) in a pressurized vessel for A) the incompressible HGO model, and B) the compressible MA model. Results are similar to those presented in Figure 5.8.
Bibliography


Chapter 6

Non-uniform hardening plasticity models for the mechanical behaviour of trabecular bone

Abstract

The inelastic behaviour of trabecular bone is established using both mechanical testing and microstructural finite element models. Continuum level constitutive models are used to capture the inelastic mechanical behaviour observed in the above \textit{in vitro} and \textit{in silico} tests.

A series of torsion tests on cylindrical specimens of trabecular bone are performed to determine its inelastic mechanical behaviour under shear loading, these data are supplemented by the uniaxial and confined compression experimental data from a previous study. An isotropic Crushable-Foam plasticity model with isotropic hardening (CFIH model) is first used to model the inelastic experimental data. This formulation is shown to be incapable of predicting the post-yield behaviour behaviour over the full range of multiaxial loading tests. A novel hardening function
is then formulated in which the hardening rate is a function of the deviatoric and volumetric plastic strain (CFMD model). This model more accurately predicts the multiaxial post-yield behaviour.

Next, micro-structural finite element models are used to test an 8 mm cube of trabecular bone in uniaxial compression, confined compression, and simple shear. An anisotropic pressure-dependent yield function with uniform hardening (XH04 model) is introduced to simulate the anisotropic inelasticity of the tissue. The XH04 model fails to predict the mode-dependent hardening observed in the micro finite element tests. A non-uniform hardening model which uses plastic-data functions to determine evolution of the yield function (XH05 model) is next used to simulate the post-yield behaviour. It is demonstrated that a coupled hardening XH05 model generates significant strain hardening and gives the best prediction of multiaxial behaviour. Finally, it is shown that the inclusion of finite deformations results in a further improvement of the prediction of multiaxial inelastic behaviour.

Nomenclature

\[
\begin{align*}
\mathbf{ab} = \mathbf{c} & \Rightarrow a_{ij} b_{jk} = c_{ik} \\
\mathbf{a} \otimes \mathbf{b} = \mathbf{c} & \Rightarrow a_i b_j = c_{ij} \\
\mathbf{a} : \mathbf{b} = \mathbf{c} & \Rightarrow a_{ij} b_{ij} = c \text{ (summation over } ij) \\
\mathbf{A} : \mathbf{b} = \mathbf{c} & \Rightarrow A_{ijkl} b_{kl} = c_{ij}. \\
\mathbf{a}' & = a_{ij} - (1/3)a_{kk} \delta_{ij}
\end{align*}
\]

6.1 Introduction

Trabecular bone is a complex highly porous material which consists of a structural system of rods and plates. It is often regarded as an open-celled foam material with pore sizes on the order of 1 mm (Keaveny et al., 2001; Cowin, 2001).

When subjected to large mechanical compressive loads, either through physical
trauma or device implantation, trabecular bone exhibits three distinct phases of inelastic mechanical behaviour (Charlebois et al., 2010b; Gibson, 2005). Firstly, a stiff elastic phase occurs where the trabecular microstructure undergoes elastic bending and compression. This is followed by a yield point where plastic buckling of the cellular structure commences. This phase exhibits an approximately constant stress with increasing strain. Finally, the cells fully collapse and the stiffness increases as the crushed foam material begins to behave like a solid. This increase in stiffness is known as densification.

In addition to plastic mechanical behaviour, trabecular bone exhibits anisotropic elasticity, damage, and visco-elastic behaviour (Keaveny et al., 1994, 2001; Linde et al., 1991). Several yield surfaces have been identified using both experimental and micromechanical finite element (micro-FE) methods (Chevalier et al., 2007; Fenech and Keaveny, 1999; Rincón-Kohli and Zysset, 2009; Sanyal et al., 2015; Wolfram et al., 2012). These studies show that trabecular bone has an anisotropic pressure-dependent yield surface.

While micro-FE models provide an excellent platform for repeatable and accurate virtual mechanical tests (Niebur et al., 2000; Sanyal et al., 2015; Nawathe et al., 2015), they are computationally expensive and infeasible for the simulation of medical devices implantation. Continuum plasticity models offer an excellent alternative to micro-FE models, provided they accurately model the full range of multiaxial mechanical behaviour exhibited by the material.

Despite the evidence of the pressure-dependent yield of trabecular bone, several studies model its inelastic using a pressure-independent von Mises plasticity formulation (Lotz et al., 1991; Mengoni et al., 2012; Mullins et al., 2009; Keyak and Rossi, 2000; Keyak, 2001). Other studies model plasticity using Drucker-Prager (Bessho et al., 2007; Carnelli et al., 2010, 2011; Mercer et al., 2006; Mullins et al., 2009) or Mohr-Coulomb (Tai et al., 2006; Wang et al., 2008) models. These friction-based
models, while strictly speaking are pressure-dependent, are intended for the material modelling of soils. In the case of DP and MC models, an increase in hydrostatic pressure stress inhibits yielding, whereas experimental data demonstrates that an increase in hydrostatic stress promotes material yielding (Kelly and McGarry, 2012). Instead, Kelly and McGarry (2012) recommend that a Crushable-Foam type model (Deshpande and Fleck, 2000) with isotropic hardening (CFIH model) to predict inelastic behaviour, and demonstrate its efficacy in modelling both uniaxial and confined compression mechanical behaviour.

This paper begins by introducing the general framework for plasticity in Section 6.2. In Section 6.3 the numerical, algorithmic implementation of this theoretical framework is presented.

In Section 6.4 of the current paper, torsion tests are performed to determine the inelastic behaviour of trabecular bone when subjected to a shear mode of loading. The uniaxial and confined compression results of Kelly and McGarry (2012) are used to supplement this shear data. It is demonstrated that the CFIH model cannot accurately predict shear behaviour. This motivates the formulation of a novel mode-dependent hardening function for the Crushable-Foam model (CFMD model). In the current paper the importance correctly modelling the post-yield hardening behaviour is highlighted, as well as using the correct yield function.

In Section 6.5 micro-FE models are used to elucidate the multiaxial anisotropic inelastic behaviour trabecular bone. Two continuum plasticity formulations featuring anisotropic yield functions are used to model the multiaxial behaviour determined in the micro-FE models. The first formulation, presented by Xue and Hutchinson (2004), uses an anisotropic pressure-dependent yield function and a uniform hardening function (XH04 model). The second formulation, also presented by Xue et al. (2005), also features an anisotropic pressure-dependent yield function but uses direction-dependent non-uniform hardening functions (XH05 model). The
incorporation of the XH05 model into a finite deformation plasticity formulation is
discussed.

Finally, in Section 6.6 the overall results of the study are discussed together with
some concluding remarks.

6.2 Theoretical Framework

6.2.1 Fundamental equations

Under the assumption of small strain linear elasticity, and additive decomposition
of the strain tensor into elastic and plastic components, the increment of the stress
tensor may be written as,

\[ d\sigma = C^e : d\varepsilon^e = C^e : (d\varepsilon - d\varepsilon^p) \] (6.1)

where \( d\varepsilon, d\varepsilon^e, d\varepsilon^p \) are the total, elastic, and plastic strain tensors respectively. \( C^e \) is
the fourth order elasticity tensor. The yield criterion for general isotropic hardening
plasticity is described as,

\[ F = f_y(\sigma) - \kappa(\varepsilon^p) = 0 \] (6.2)

where \( f_y(\sigma) \) is the yield function, which is a function of the stress tensor. The
function, \( f_y(\sigma) \), must be chosen carefully as it must be able to adequately represent
the yielding of the material being modelled under a multi-axial stress state. The
hardening function, \( \kappa(\varepsilon^p) \), is a function of the plastic strain tensor. However it
is commonly assumed to be a function of the equivalent plastic strain, \( \varepsilon_{eq}^p \), which
reduces it to the scalar function \( \kappa(\varepsilon_{eq}^p) \). This describes the equivalent stress-strain
behaviour of the material. In the course of this study different yield functions and hardening functions will be examined to assess their suitability for modelling trabecular bone as a continuum material.

Assuming the general case of a non-associated flow rule, the increment of plastic strain is defined by the equation

$$d\varepsilon_p = d\lambda \frac{df_p(\sigma)}{d\sigma}$$  \hspace{1cm} (6.3)

where $f_p(\sigma)$ is the plastic potential function, and $d\lambda$ is the plastic multiplier. In the specific case of associated flow, the plastic potential function is equal to the yield function ($f_p(\sigma) \equiv f_y(\sigma)$). Both $f_y(\sigma)$ and $f_p(\sigma)$ must be continuously differentiable functions of the stress. The equivalent plastic strain $\varepsilon_{eq}^p$ is defined using the principal of plastic work equivalence (Cvitanić et al., 2008),

$$f_y(\sigma) d\varepsilon_{eq}^p = \sigma : d\varepsilon^p$$ \hspace{1cm} (6.4)

The increment of equivalent plastic strain is commonly rewritten using (6.3), (6.4), and Euler’s identity for first order homogeneous functions,

$$d\varepsilon_{eq}^p = d\lambda \frac{f_p(\sigma)}{f_y(\sigma)}$$ \hspace{1cm} (6.5)

In the case of associated flow the increment of equivalent plastic strain is equal to the plastic multiplier, $d\varepsilon_{eq}^p = d\lambda$.

The Kuhn-Tucker conditions are based on the criteria for plastic loading and
elastic unloading, they state that,

\[ d\lambda \geq 0, \quad F \leq 0, \quad d\lambda F = 0. \quad (6.6) \]

In plastic loading \( dF = 0 \), leading to the consistency condition

\[ d\lambda dF = 0 \quad (6.7) \]

The consistency condition is used to obtain differential equations for the stress and plastic strain. Assuming isotropic hardening, differentiating (6.2) and using (6.7) leads to,

\[ dF = \frac{\partial F}{\partial \sigma_{ij}} \dot{\sigma}_{ij} + \frac{\partial F}{\partial \kappa} \dot{\kappa} = 0 \quad (6.8) \]

leading to

\[ \frac{\partial f_y}{\partial \sigma} : d\sigma - \frac{d\kappa}{d\varepsilon_{eq}} d\varepsilon_{eq} = 0 \quad (6.9) \]

Inserting (6.3) into (6.2) and substituting this expression into (6.9) we can obtain an explicit expression for the plastic multiplier increment \( d\lambda \):

\[ d\lambda = \frac{\frac{\partial f_y}{\partial \sigma} : \mathbf{C}^e : d\varepsilon}{\frac{d\kappa}{d\varepsilon_{eq}} \int_p + \frac{\partial f_y}{\partial \sigma} : \mathbf{C}^e : \frac{\partial f_y}{\partial \sigma}} \quad (6.10) \]

A numerical implementation of the constitutive equations above is outlined in
6.2.2 Finite deformation plasticity

In cases where elastic strains exceed 1-2%, the infinitesimal strain assumption in standard plasticity formulations is no longer valid. Hyper-plastic formulations have been developed which overcome the known issues regarding anisotropic hypoelastic plasticity models. These models are based on hyperelastic relations and a multiplicative split of the deformation gradient into elastic and plastic components. Specifically we adopt the modular formulation previously outlined in Miehe et al. (2002), Caminero et al. (2011) and Montáns et al. (2012) whereby a small-strain plasticity formulation may be used in conjunction with a geometric pre-processor and post-processor to ensure that the solution is consistent with the finite deformation mechanics.

6.2.2.1 Kinematics and deformation

In small strain plasticity the incremental strain is additively decomposed into elastic and plastic parts (see (6.1)). In large strain plasticity, elastic and plastic deformations are modelled by multiplicatively splitting the deformation gradient into elastic and plastic parts (Lee, 1969). The deformation gradient, $\mathbf{F}$, from the undeformed configuration at time 0 to a deformed configuration at time $t$ is,

$$\mathbf{F}_{\tau} = \mathbf{F}_{\tau}^e \mathbf{F}_{\tau}^p,$$

where $\tau$ is the intermediate configuration where the elastic deformation has been removed, i.e. it is a stress-free configuration. As only plastic deformations occur from time $0 \rightarrow \tau$, and only elastic deformations occur from time $\tau \rightarrow t$, $\mathbf{F}_{\tau}^e = \mathbf{F}_{\tau}^e$ and $\mathbf{F}_{\tau}^p = \mathbf{F}_{\tau}^p$. A schematic of the multiplicative decomposition of the deformation
gradient is shown in Figure 6.1. The total Eulerian (deformed) velocity gradient \( l = \partial \mathbf{v} / \partial \mathbf{x} \) may be written in terms of the deformation gradient (dropping the pre-scripts) as,

\[
l = \dot{\mathbf{F}} \mathbf{F}^{-1}. \tag{6.12}
\]

This in turn may be written in terms of the elastic and plastic deformation gradients as,

\[
l = l^e + l^p = \dot{\mathbf{F}}^e \mathbf{F}^e + \mathbf{F}^e (\dot{\mathbf{F}}^p \mathbf{F}^{p-1}) \mathbf{F}^{e-1}. \tag{6.13}
\]

The term in brackets is the modified plastic velocity gradient \( L^p \),

\[
L^p = \dot{\mathbf{F}}^p \mathbf{F}^{p-1}, \tag{6.14}
\]

which exists in the intermediate configuration. The tensor \( L^p \) may be additively split into symmetric and and skew-symmetric parts, \( D^p \) and \( \mathbf{W}^p \), the plastic deformation rate and plastic spin respectively. In cases where rotations are accounted for by using a local-coordinate system (Caminero et al., 2011; Hosseini et al., 2015) the plastic spin may be neglected, \( \mathbf{W}^p = \mathbf{0} \), then the velocity gradient may be approximated as the modified plastic deformation rate tensor \( D^p \),

\[
L^p \approx D^p \tag{6.15}
\]
Combining (6.14) and (6.15) the rate of the plastic deformation gradient tensor is,

\[ \dot{F}^p = D^p F^p, \quad (6.16) \]

The plastic deformation gradient may be updated using,

\[ t^+\Delta t \dot{F}^p_0 = \exp(\Delta t^t+\Delta t^t D^p) \dot{F}^p_0 \quad (6.17) \]

The following updates to the elastic and plastic deformation gradients may be calculated using (6.17) and the definition (6.11),

\[ t^+\Delta t \dot{F}^e = F^e_* \exp(-\Delta t^t+\Delta t^t D^p) \quad (6.18) \]

\[ (t^+\Delta t \dot{F}^p_0)^{-1} = (\dot{F}^p_0)^{-1} \exp(-\Delta t^t+\Delta t^t D^p) \quad (6.19) \]

where \( F^e_* = t^+\Delta t \dot{F}^e_0 \) is the trial elastic deformation gradient. The trial deformation tensor is defined as \( C^e_* = F^e_*^T F^e_* \). Using this definition and (6.18),

\[ C^e_* = \exp(\Delta t^t+\Delta t^t D^p) t^+\Delta t \dot{C}^e \exp(\Delta t^t+\Delta t^t D^p) \quad (6.20) \]
The logarithmic (Hencky) strain $\varepsilon_{\text{log}}$ is defined in terms of the deformation tensor as,

$$\varepsilon_{\text{log},*}^{*} = \frac{1}{2} \ln C_{*}^{e},$$

(6.21)

$$t^{+}\Delta t^{c}_{\text{log}} = \frac{1}{2} \ln t^{+}\Delta t_{0}^{c},$$

(6.22)

Using the definitions (6.21) and (6.22), (6.20) is rewritten as,

$$t^{+}\Delta t^{c}_{0} \approx \varepsilon_{\text{log},*}^{e} - \Delta t^{+}\Delta t^{*}_{0} \mathbf{D}^{p},$$

(6.23)

with the proviso that the elastic strains and the incremental step are only moderately large.

6.2.2.2 Strain energy function and stress measures

A strain energy function for anisotropic elasticity is proposed based on the logarithmic strain (Caminero et al., 2011; Montáns and Bathe, 2005, 2007).

$$W = \frac{1}{2} \varepsilon_{\text{log}}^{e} : \mathbf{C}^{e} : \varepsilon_{\text{log}}^{e}.$$  

(6.24)

where $\mathbf{C}^{e}$ is the elasticity tensor which may interpreted as having the same meaning as the small-strain elasticity tensor.

The generalized Kirchhoff stress tensor is defined in the intermediate configura-
Figure 6.1: Schematic illustrating the different configurations used in the multiplicative decomposition of the deformation gradient, and the stress measures used for each configuration. In the intermediate configuration the elastic strains are relaxed and the body is stress-free, the plastic deformation persists. The stress update is performed in the intermediate configuration using the generalized Kirchhoff stress.

It can be shown for moderate elastic strains in anisotropic elasticity ($|\varepsilon_{\log}^e| \ll 1$) that $T$ is equal to the symmetric part of the Mandel stress tensor $\Sigma_S$ (Montáns and Bathe, 2005). In this case the total Mandel stress is determined to be,

$$\Sigma = \Sigma_S + \Sigma_W \simeq T + T_W$$

(6.26)

where $T_W$ is the skew-symmetric part of $T$. The second Piola–Kirchhoff $S$ stress

$$T = \frac{\partial W}{\partial \varepsilon_{\log}^e} = C^e : \varepsilon_{\log}^e.$$  

(6.25)
may be determined from the Mandel stress tensor as,

\[ S = C^{-1} \Sigma. \] (6.27)

Any of the common stress tensors may be determined from the second Piola–Kirchhoff stress using the standard transformations. For instance the Cauchy stress,

\[ \sigma = J^{-1} F S F^T. \] (6.28)

The advantage of the formulation above is that the fundamental equations outlined in Section 6.2.1 and their numerical implementation in Section 6.3.1 may be used to calculate the stress-update in the intermediate configuration. All that is required is that some straightforward substitutions are made: \( \sigma = T \) for the stress, and \( d\varepsilon^p = \Delta t^{t^* + \Delta t} D^p \) for the increment of plastic strain. It is also necessary that the yield and hardening functions be formulated in the intermediate configuration using generalized Kirchhoff stress–log strain space, rather than Cauchy stress–log strain space. This can be easily achieved using the conversion,

\[ T = J F^T \sigma F^{-T}. \] (6.29)

The precise methodology for implementation of the finite deformation plasticity formulation is outlined in Section 6.3.2.
6.3 Numerical Implementation

The equations for the constitutive model outlined in Section 6.2 are non-linear and a numerical scheme is required for their solution. This section outlines an algorithm to calculate an increment of stress given an increment of strain and the state-dependent variables of the previous increment. Additionally, an algorithm for implementation of the finite strain plasticity is presented. Finally, a numerical method to calculate the elasto-plastic tangent matrix, which is required for implementation of the plasticity model in implicit finite element schemes, is outlined.

6.3.1 Predictor-corrector algorithm

The increment of stress is given by Equation (6.1) and is written algorithmically as,

\[ \Delta \sigma = C^e : (\Delta \varepsilon - \Delta \varepsilon^p) \]  

(6.30)

To determine the stress increment an initial guess is made that the increment is fully elastic. This is known as the predictor step. The trial stress \( \sigma^{tr} \) is calculated for the increment \( t + \Delta t \) using,

\[ \sigma^{tr} = \sigma^t + C^e : \Delta \varepsilon \]  

(6.31)

where \( \sigma^t \) is the stress at time \( t \). Next the yield criterion (6.2) is tested, and if \( F > 0 \) then a plastic corrector step is initiated which calculates \( \Delta \varepsilon^p \) such that (6.2) is satisfied. The final stress is given by,

\[ t + \Delta t \sigma = \sigma^{tr} - C^e : \Delta \varepsilon^p \]  

(6.32)
Using equations (6.2), (6.3), (6.5), (6.7), and (6.32) the following residual equations are defined (Cvitanic et al., 2008).

\[
\begin{align*}
\Phi_1 &\equiv f(\sigma) - \rho \\
\Phi_2 &\equiv C^{-1} : (\sigma - \sigma^t) + \Delta \lambda v = 0 \\
\Phi_3 &\equiv \rho - \kappa(\varepsilon^p) = 0 \\
\Phi_4 &\equiv f_y(\sigma) \Delta \varepsilon_{eq}^p + f_p(\sigma) \Delta \lambda = 0
\end{align*}
\]

where \( \Phi_2 \) is a second order tensor and the other residuals are scalars, \( v = \frac{\partial f_p(\sigma)}{\partial \sigma} \), and \( \rho \) is the current value of the scalar hardening function. The above residuals may be solved incrementally for the unknowns \( \sigma_{n+1}, \rho_{n+1}, \Delta \varepsilon_{eq}^p, \) and \( \Delta \lambda \) using a Newton-Raphson method. Firstly the residuals \( \Phi_1-\Phi_4 \) must be linearised.

\[
\begin{align*}
\Phi_1 + w : \Delta \sigma - \Delta \rho &= 0 \\
\Phi_2 + C^{-1} : \Delta \sigma + \Delta \lambda (\partial v / \partial \sigma) : \Delta \sigma + \delta \Delta \lambda v &= 0 \\
\Phi_3 + \Delta \rho - (d\kappa / d\varepsilon_{eq}^p) \delta \Delta \varepsilon_{eq}^p &= 0 \\
\Phi_4 + (\Delta \varepsilon_{eq}^p w - \Delta \lambda v) : \Delta \sigma + f_y \delta \Delta \varepsilon_{eq}^p - f_p \delta \Delta \lambda &= 0
\end{align*}
\]
where $w = \partial f_y(\sigma) / \partial \sigma$. Analytical expressions for updates to the solution variables are given by inversion and simplification of Equations (6.37)–(6.40).

\[
\delta \Delta \varepsilon_{eq}^p = \frac{\Phi_1 - w : M^{-1} : \Phi_2 - (\Phi_4/f_p)w : M^{-1} : v + \Phi_3}{(d\kappa/d\varepsilon_{eq}^p) + (f_y/f_p)w : M^{-1} : v}
\] (6.41)

\[
\Delta \sigma = -M^{-1} : (\Phi_2 + f_p(\Phi_4 + f_y \delta \Delta \varepsilon_{eq}^p)v)
\] (6.42)

\[
\delta \Delta \lambda = (\Phi_4 + G : \Delta \sigma + f_y \delta \Delta \varepsilon_{eq}^p)/f_p
\] (6.43)

\[
\Delta \rho = -\Phi_3 + (d\kappa/d\varepsilon_{eq}^p)\delta \Delta \varepsilon_{eq}^p
\] (6.44)

where $\bar{C} = C^e - 1 + \Delta \lambda (\partial \nu / \partial \sigma)$, $G = \Delta \varepsilon_{eq}^p w - \Delta \lambda v$, and $M = \bar{C} + v \otimes G / f_p$. The variables are updated at each increment $n$ as follows,

\[
\Delta \varepsilon_{eq}^{p(n+1)} = \Delta \varepsilon_{eq}^{p(n)} + \delta \Delta \varepsilon_{eq}^{p(n)}
\] (6.45)

\[
\Delta \lambda^{(n+1)} = \Delta \lambda^{(n)} + \delta \Delta \lambda^{(n)}
\] (6.46)

\[
\sigma^{(n+1)} = \sigma^{(n)} + \Delta \sigma^{(n)}
\] (6.47)

\[
\rho^{(n+1)} = \rho^{(n)} + \Delta \rho^{(n)}
\] (6.48)

This increment is then checked for yielding using the $\Phi_1$ residual given in (6.33). If the absolute value of $\Phi_1$ is less than a predefined tolerance, then that increment is judged to have arrived at a converged solution for the increment of stress. If this is not the case, then another iteration is performed. The stress update algorithm given above has been outlined in Table 6.1.

### 6.3.2 Finite deformation implicit stress update algorithm

This section outlines the numerical implementation of the finite deformation plasticity model given in Section 6.2.2. The plasticity step itself is solved in the intermediate
Table 6.1: Infinitesimal strain based stress update algorithm for the plasticity formulation with implicit return mapping scheme.

1. Import state dependent variables from previous increment: stress \( \sigma \); equivalent stress \( \rho \); equivalent plastic strain \( \varepsilon_{eq}^{p} \); volumetric plastic strain \( \varepsilon_{vol}^{p} \); deviatoric plastic strain \( \varepsilon_{dev}^{p} \).

2. Calculate elastic trial stress \( \sigma^{tr} \).

3. Initialise incremental variables: \( n = 1 \)

4. Check for yield: \( \Phi^{(n)}_{1} = f(\sigma^{(n)}) - \rho^{(n)} \)
   - Yes: Elastic deformation, \( \sigma_{t+\Delta t} = \sigma^{(n)} \). EXIT
   - No: Plastic deformation. Continue.

5. Compute the residuals: \( \Phi^{(n)}_{2} \), \( \Phi^{(n)}_{3} \), and \( \Phi^{(n)}_{4} \).

6. Compute the incremental change in plastic strain \( \delta \varepsilon_{eq}^{p(n)} \).

7. Compute the increments: \( \Delta \sigma^{(n)} \), \( \delta \Delta \lambda^{(n)} \), \( \Delta \rho^{(n)} \).

8. Update the state variables: \( \sigma^{(n+1)} \), \( \Delta \lambda^{(n+1)} \), \( \Delta \varepsilon_{eq}^{p(n+1)} \), \( \rho^{(n+1)} \).

9. Check for convergence:
   (i) Compute \( \Phi^{(n+1)}_{1} \) using updated variables
   (ii) Check criteria: \( \Phi^{(n+1)}_{1} \leq \text{tol} \)
      - Yes. Converged solution: \( t+\Delta t \sigma = \sigma^{(n+1)} \); \( t+\Delta t \rho = \rho^{(n+1)} \);
      - No. \( n = n + 1 \). Go to item 4. EXIT.
configuration and then transformed to the spatial configuration. This involves three main steps (Miehe et al., 2002; Caminero et al., 2011): a geometric pre-processor, a predictor-corrector algorithm, and a geometric post-processor.

6.3.2.1 Geometric pre-processor:

For a given increment of deformation/strain, the trial elastic state must be computed. If the elastic state violates the yield criterion, then a plastic correction must be computed. For finite deformations with a multiplicative split of the deformation gradient into elastic and plastic components, the trial elastic deformation gradient, $F_e^*$, is determined using the total deformation gradient at $t + \Delta t$ and the plastic deformation gradient at $t$,

$$F_e^* = F_{t + \Delta t}^p F_{t}^p - 1. \quad (6.49)$$

Next, the trial Cauchy–Green deformation tensor $C_e^*$ must be computed,

$$C_e^* = F_e^{*T} F_e^* = \sum_{i=1}^{3} (\lambda_{e_i}^2) n_{e_i} \otimes n_{e_i}, \quad (6.50)$$

where spectral decomposition of $C_e^*$ has been used to determine the trial principal stretches $\lambda_e$ and their directions $n_e$. The trial elastic logarithmic strain tensor $\varepsilon_{\log, e}^*$ is determined using,

$$\varepsilon_{\log, e}^* = \frac{1}{2} \ln C_e^* = \sum_{i=1}^{3} \ln(\lambda_{e_i}) n_{e_i} \otimes n_{e_i}. \quad (6.51)$$
Using the trial elastic logarithmic strain the trial generalized Kirchhoff stress $T_*$ is determined:

$$T_* = \frac{\partial W}{\partial \varepsilon_{\log,*}^e} = C^e : \varepsilon_{\log,*}^e.$$

(6.52)

The trial elastic log strain and the generalized Kirchhoff stress may now be input into a small-strain algorithm to determine plastic strain increment.

The above procedure has been summarised in Table 6.2.

### 6.3.2.2 Predictor-corrector algorithm

Using the trial elastic state, a predictor-corrector algorithm framed in the intermediate configuration is used to determine the stress $T$, the plastic strain increment $\Delta^t D_p$, the equivalent stress $\rho$, and the deviatoric and volumetric plastic strains $\varepsilon_p^{dev}$ and $\varepsilon_p^{vol}$ at $t + \Delta t$. The theoretical framework for this algorithm is presented in Section 6.2.1. Its numerical implementation is outlined in Section 6.3.1 and summarised in Table 6.1.

### 6.3.2.3 Geometric post-processor

The plastic corrector step determines the plastic strain increment and generalized Kirchhoff stress at $t + \Delta t$. The elastic log strain is calculated using (6.23) and spectral decomposition is performed on the resultant tensor,

$$\varepsilon_{\log}^e = \varepsilon_{\log,*}^e + \tau^t \Delta t \Delta \varepsilon_p = \sum_{i=1}^{3} \xi_i m_i \otimes m_i,$$

(6.53)
where \( \xi_i \) are the eigenvalues and \( \mathbf{m}_i \) the corresponding eigenvectors of \( \varepsilon_{\text{log}}^e \). The elastic Cauchy–Green deformation tensor is calculated using,

\[
C^e = \sum_{i=1}^{3} \exp(2\xi_i) \mathbf{m}_i \otimes \mathbf{m}_i.
\] (6.54)

The symmetric part of the Mandel stress is equal to the generalized Kirchhoff stress,

\[
\Sigma_S = \mathbf{T},
\] (6.55)

the skew-symmetric part of the Mandel stress is given as,

\[
\Sigma_W = \varepsilon_{\text{log}}^e \mathbf{T} - \mathbf{T} \varepsilon_{\text{log}}^e,
\] (6.56)

and the total Mandel stress is given as,

\[
\Sigma = \Sigma_S + \Sigma_W.
\] (6.57)

Using the elastic Cauchy–Green deformation tensor and the Mandel stress, the second Piola–Kirchhoff stress is,

\[
\mathbf{S} = \frac{1}{2} \left( \Sigma (C^e)^{-1} + (C^e)^{-1} \Sigma \right).
\] (6.58)

where this form has been used to ensure that \( \mathbf{S} \) is symmetric. Finally, the Cauchy
stress is given by the standard transformation,

\[ \sigma = J^{-1} F S F^T. \] (6.59)

The plastic deformation gradient is calculated for use in the next plastic step,

\[ t^{+\Delta t} F^{p(-1)} = t^{F(-1)} \exp(-\Delta t D^p) \] (6.60)

The above procedure has been summarised in Table 6.3.

### 6.3.3 Numerical Consistent Tangent Matrix

For implicit FE schemes the tangent matrix must be computed and returned to the FE solver. The current study uses the FE software Abaqus, which requires the Jaumann rate of the spatial consistent tangent matrix (Prot et al., 2007),

\[ \mathbf{c}_{ijkl} \equiv \mathbf{c}_{ijkl} + \frac{1}{2}(\delta_{ik}\sigma_{jl} + \sigma_{ik}\delta_{jl} + \delta_{il}\sigma_{jk} + \sigma_{il}\delta_{jk}) \] (6.61)

where \( \mathbf{c}_{ijkl} \) is the fourth order spatial elasticity tensor given by,

\[ \mathbf{c} = 4J^{-1}\mathbf{b} \frac{\partial^2 \Psi(\mathbf{b})}{\partial \mathbf{b} \partial \mathbf{b}} \mathbf{b}. \] (6.62)

where \( \mathbf{b} \) is the left Cauchy-Green deformation tensor, and \( \Psi(\mathbf{b}) \) is the strain energy density function. A numerical method is implemented in the current study to calculate the consistent tangent matrix. The starting point is the Jaumann rate of the
Table 6.2: Geometric pre-processor for finite deformation plasticity formulation

1. Input data: deformation gradient $t + \Delta t \mathbf{F}$; inverse plastic deformation gradient $t \mathbf{F}^{-1}$; material parameters $\Lambda$.

2. Trial deformation gradient: $\mathbf{F}^e = t + \Delta t \mathbf{F} \mathbf{F}^{-1}$

3. Trial elastic Cauchy–Green deformation tensor: $\mathbf{C}^e = \mathbf{F}^e \mathbf{F}^{e T} = \sum_{i=1}^{3} (\lambda_i^2) \mathbf{n}_i \otimes \mathbf{n}_i$

4. Trial elastic log strain in undeformed configuration: $\varepsilon_{\text{log},e}^e = \sum_{i=1}^{3} \ln(\lambda_i) \mathbf{n}_i \otimes \mathbf{n}_i$

5. Trial generalized Kirchhoff stress: $\mathbf{T}^e = \partial W / \partial \varepsilon_{\text{log},e}^e$

Table 6.3: Geometric post-processor algorithm for finite-strain implicit plasticity constitutive model.

1. Elastic log strain: $\varepsilon_{\text{log}}^e = \varepsilon_{\text{log},e}^e - t + \Delta t \varepsilon_p = \sum_{i=1}^{3} \xi_i \mathbf{m}_i \otimes \mathbf{m}_i$

2. Cauchy–Green deformation tensor: $\mathbf{C}^e = \sum_{i=1}^{3} \exp(2 \xi_i) \mathbf{m}_i \otimes \mathbf{m}_i$

3. Symmetric Mandel stress: $\Sigma_S = \mathbf{T}$

4. Skew-symmetric Mandel stress: $\Sigma_W = \varepsilon_{\text{log}}^e \mathbf{T} - \mathbf{T} \varepsilon_{\text{log}}^e$

5. Mandel stress: $\Sigma = \Sigma_S + \Sigma_W$

6. Second Piola–Kirchhoff stress: $\mathbf{S} = \frac{1}{2} \left( \mathbf{\Sigma} \mathbf{C}^{e(-1)} + \mathbf{C}^{e(-1)} \mathbf{\Sigma} \right)$

7. Cauchy stress: $\sigma = J^{-1} \mathbf{F} \mathbf{S} \mathbf{F}^T$

8. Plastic deformation gradient: $t + \Delta t \mathbf{F}^{p(-1)} = t \mathbf{F}^{p(-1)} \exp(-\Delta \varepsilon_p)$
Kirchhoff stress,

\[ \nabla \tau = \dot{\tau} - w\tau - \tau w = C^{r_J} : D \]

(6.63)

where \( C^{r_J} \) is the tangent matrix for the Jaaumann rate of the Kirchhoff stress. The numerical approximation for the consistent tangent matrix is determined using a forward difference perturbation method,

\[ \nabla \epsilon^{(ij)} \approx \frac{1}{J\epsilon} \left[ \tau(\hat{F}^{(ij)}) - \tau(F) \right] \]

(6.64)

where \( \epsilon \) is a dimensionless perturbation increment, \( \tau(\hat{F}^{(ij)}) \) is the perturbed Kirchhoff stress for a perturbation \( (ij) \), and \( \tau(F) \) is the Kirchhoff stress. The perturbed Kirchhoff stress is computed by calculating the Kirchhoff stress using the perturbed deformation gradient \( \hat{F}^{(ij)} \) where,

\[ \hat{F}^{(ij)} = F + \Delta F^{(ij)} \]

(6.65)

and

\[ \Delta F^{(ij)} = \frac{\epsilon}{2} \left[ (e_i \otimes e_j)F + (e_j \otimes e_i)F \right] \]

(6.66)

where \( e_i \) for \( i = \{1, 2, 3\} \) are the basis vectors in the spatial description. To calculate the \( 6 \times 6 \) consistent tangent matrix \( (\text{DDSDDE in Abaqus}) \) a \( 6 \times 1 \) perturbed Kirchhoff stress \( \tau(\hat{F}^{(ij)}) \) in Voigt notation is computed six times for each \( (ij) = \{11, 22, 33, 12, 13, 23\} \) and using (6.64) to calculate the total matrix. The
The above numerical algorithm comes at a considerable computational cost, as the stress must be calculated seven times, once for $\mathbf{F}$ and for each $\hat{\mathbf{F}}^{(ij)}$. However, it does expedite the creation of custom material models, and is particularly useful in the context of this study where we are dealing with finite deformation plasticity.
6.4 Mode-Dependent Strain Hardening

In this section the inelastic behaviour of trabecular bone under multiaxial loading is investigated. As a starting point the isotropic Crushable-Foam yield function presented by Deshpande and Fleck (2000) is used to model the plasticity of the material. Following from this, a novel hardening function which changes hardening rate depending on the volumetric and deviatoric loading is introduced.

6.4.1 Multiaxial mechanical tests on trabecular bone

In order to characterise the multiaxial yield and hardening behaviour of trabecular bone, Kelly and McGarry (2012) undertook a series of uniaxial compression and confined compression experiments on 8 mm cube specimens of bovine trabecular bone up to large strains. A schematic of the boundary conditions for these two experiments is outlined in Figure 6.2A and B. In uniaxial compression a displacement \( u_3 \) is applied to the top face of the cube in the 3-direction, the cube is free to displace in the 1- and 2-directions. In confined compression a displacement \( u_3 \) is applied to the top face, in this case no lateral expansion is permitted and the specimen is constrained from displacing in the 1- and 2-directions.

Additionally, a series of torsion experiments are performed on bovine trabecular bone to determine its yield and hardening behaviour under shear loading. The protocol from Ford and Keaveny (1996) for specimen preparation and mechanical testing is adopted. A schematic of the experiment is outlined in Figure 6.2C. A rotation, \( \theta \), is applied to the top face of the cylindrical specimen up to an angle of \( \pi/4 \) or failure, and the torque is measured throughout. A total of five specimens are tested. The shear stress \( \sigma_{13} \) in an infinitesimal element on the surface of the
specimen is determined using the equation (Nadai, 1950),

$$\sigma_{13} = \frac{1}{2\pi r^3} \left[ \bar{\theta} \frac{dT}{d\theta} + 3T \right]$$

(6.67)

where $T$ is the torsion, $r$ the radius of the specimen, $\bar{\theta}$ is the angle of twist per unit height.

The shear stress-strain curve for the torsion experiment is given in Figure 6.3A, and shows the mean and standard deviation. The 0.2% offset yield stress is 3.81 MPa and the shear modulus 136.07 MPa. This result for the shear behaviour is presented alongside the uniaxial and confined compression stress-strain plots in Figure 6.3B. It should be noted that the post-yield hardening rate is different for each of the loading scenarios examined.

### 6.4.2 Prediction of multiaxial stress-strain behaviour using a Crushable-Foam model

The importance of using a pressure-dependent yield function to model the multiaxial plastic behaviour of trabecular bone has previously been highlighted (Kelly and McGarry, 2012), and is vital for the accurate simulation of orthopaedic medical device implantations using FE analysis (Kelly et al., 2013a,b; Kinzl et al., 2013). Though the Mohr-Coulomb and Drucker-Prager plasticity formulations feature a pressure-dependent yield function, material yielding is inhibited by an increase in hydrostatic stress in such friction based formulations. As a result, Mohr-Coulomb, Drucker-Prager, and indeed von Mises yield functions fail to capture experimentally observed plasticity under confined compression loading (it should be noted, the von Mises plasticity is analogous to Mohr-Coulomb or Drucker-Prager plasticity with a friction angle of 0°). In contrast, Kelly and McGarry (2012) determined that the
Figure 6.2:  A) Schematic of the boundary conditions for the uniaxial compression test of a cubic specimen of trabecular bone. A displacement $u_3$ is applied in the $3$-direction, the cube is free to expand in the $1$- and $2$-directions. B) Schematic of the boundary conditions for the confined compression test of a cube specimen. A displacement $u_3$ is applied in the $3$-direction, the cube is not permitted to expand in the $1$- and $2$-directions. C) Schematic outlining the boundary conditions for the torsion test. The bottom face of a cylinder is fixed and a rotation $\theta$ is applied to the top face. The torque is measured throughout, and (6.67) is used to calculate the shear stress at the surface of the cylinder.
Figure 6.3: A) Nominal mean shear stress-strain curve determined from the torsion experiments ($n = 5$). The error bars indicate the standard deviation. B) Plot of the mean stress-strain curves from the confined compression, uniaxial compression, and torsion experiments. Note the secondary axes used for the torsion experiment.

An isotropic pressure-dependent plasticity constitutive model by Deshpande and Fleck (2000) for isotropic cellular solids can accurately capture the yielding observed in a confined compression experiment. The key feature of the formulation is that an increase in hydrostatic stress promotes material yielding. Indeed the study by Kelly et al. (2013b) suggest that trabecular bone, like many cellular solids, can yield under pure hydrostatic stress.

The yield function for this model, sometimes called the Crushable-Foam (CF) model, is given as,

$$f_y(\sigma) = \left\{ \frac{1}{(1 + (\alpha/3)^2)} \left[ q^2 + \alpha^2 p^2 \right] \right\}^{1/2}$$  \hspace{1cm} (6.68)

where the von Mises stress $q = \sqrt{(3/2)\sigma' : \sigma'}$, the pressure stress $p = \text{tr}(\sigma)/3$, and $\alpha$ is a material parameter which governs the shape of the yield surface, which is ellipsoidal in shape in principal stress space, elliptical in the meridional stress $(q - p)$ plane. A plot of the yield surface is shown in Figure 6.4. This yield function
Figure 6.4: Plot of the CF yield surface in principal stress space for $\alpha = 0.72$. The axes are normalised by the uniaxial yield strength $\sigma_y$. Note the ellipsoid shape of the yield surface, which predicts yielding in hydrostatic loading (blue line).

is dependent on both the deviatoric stress and the pressure (volumetric) stress, hence yield may be achieved from a deviatoric stress state, a hydrostatic stress, or a combination of deviatoric and hydrostatic stress (see Figure 6.4B).

Typically this model is used with isotropic hardening (Abaqus V6.14, 2015) where $\kappa = \kappa(\varepsilon_{eq}^p)$. This formulation is commonly referred to as the Crushable-Foam with Isotropic Hardening (CFIH model), as implemented in Kelly and McGarry (2012).

In addition to the uniaxial and confined compression experiments, the shear data from Section 6.4.1 is modelled using the parameters outlined in Kelly and McGarry (2012). For the yield function $\alpha = 0.72$ and for the plastic potential $\beta = 1.53$, the uniaxial yield stress $\sigma_y^0 = 13.2$ MPa. Linear isotropic elasticity is assumed with Young’s modulus $E = 292.13$ MPa, and Poisson’s ratio $\nu = 0.16$. The uniaxial stress–plastic strain experimental data are used for the hardening function $\kappa(\varepsilon_{eq}^p)$. Non-associated flow is used where the plastic potential function takes a similar form to the yield surface: $f_p^2(\sigma) = [q^2 + \beta^2p^2] / [1 + (\beta/3)^2]$.

Computed results are plotted alongside the corresponding experimental data in Figure 6.5. As the uniaxial data is used to calibrate the yield surface and to define the
Figure 6.5: Experimental nominal stress-strain curves, and those predicted by the CF model under confined compression, uniaxial compression, and shear loading. Note that for confined and uniaxial compression $i = 3$ is the 33 component of stress/strain, and for shear $i = 5$ is the 13 component of stress/strain. As the hardening behaviour of the CF model is defined by the uniaxial stress response, the experimental and predicted curves are identical. While the CF model is able to adequately capture the yielding and immediate post-yield of the confined compression test, it fails to fully model the hardening behaviour. Finally, the Crushable-Foam model can neither predict the correct yield, or the post-yield stress-strain behaviour of the shear experiment.
hardening behaviour, the predicted uniaxial and experimental stress-strain curves are identical. The CFIH model can accurately capture the yield point of the confined compression experiment, and the immediate post-yield behaviour. However, for strains greater than 0.1 the predicted hardening behaviour does not accurately replicate the experimental data. The increased hardening rate observed experimentally under confined compression loading is not captured by the model. An error of 51.3% at a strain of 0.4 can be observed in Figure 6.5 due to the underprediction of confined compression hardening. Finally, neither the yield nor the hardening behaviour observed in the experimental shear data is accurately predicted by the current CFIH model.

In the case of shear deformation, material yielding is a function of the von Mises stress $q$ and the parameter $\alpha$. There is no flexibility in the yield function to calibrate the model independently for deviatoric and volumetric deformations and hence the yield point in Figure 6.5 is substantially over-predicted.

The use of the CFIH model to simulate the multiaxial inelastic behaviour of trabecular bone (Kelly and McGarry, 2012) is a substantial improvement on previously used models such as the Drucker-Prager (Mercer et al., 2006) or Mohr-Coulomb (Wang et al., 2008). However, some modification of the model is required to accurately capture post-yield strain hardening of trabecular bone under multiaxial loading.

### 6.4.3 Formulation of a new hardening function

Given the shortcomings highlighted in Section 6.4.2 a new hardening function is formulated in order to accurately predict the post-yield hardening behaviour of trabecular bone observed under multiaxial loading conditions.

Recalling Figure 6.3B, the post-yield hardening rate increases as the loading mode is changed from shear, to uniaxial compression, to confined compression. In
Plot the direction of each of the loading modes examined in Section 6.4.1 in the von Mises-pressure stress \( q - p \) plane. As shear loading is entirely deviatoric, the pressure stress is zero. Uniaxial loading entails a mixture of both deviatoric and hydrostatic (pressure) loads, and \( q/p = 3 \). As lateral expansion is not permitted in confined compression, pressure stress is more dominant. The exact \( q/p \) ratio depends upon the plastic Poisson’s ratio, but in this case \( q/p = 0.92 \).

Figure 6.6 each of these loading modes is plotted in the von Mises stress–pressure stress \( q - p \) plane. As shear loading is entirely deviatoric, its path is along the \( q \) axis i.e. \( p = 0 \). Uniaxial loading consists of both deviatoric and pressure stress and results in a \( q/p = 3 \). Finally, the confined compression loading is dependent on the plastic Poisson’s ratio. For the experimental data in Section 6.4.2, \( q/p = 0.92 \).

Given the experimental observations, this implies that as the \( q/p \) ratio decreases, the post-yield hardening rate increases.

Hence, a hardening function is devised in which the deviatoric and volumetric plastic deformations are decoupled. This permits different hardening rates to be computed depending on the mode of loading. Specifically, the hardening function is a function of the deviatoric and volumetric plastic strains. It takes on the general form,

\[
\kappa(\varepsilon_{\text{vol}}^p, \varepsilon_{\text{dev}}^p) = \kappa_{\text{vol}}(\varepsilon_{\text{vol}}^p) + \kappa_{\text{dev}}(\varepsilon_{\text{dev}}^p) + \kappa_{\text{mix}}(\varepsilon_{\text{vol}}^p, \varepsilon_{\text{dev}}^p) + \kappa_{0} \tag{6.69}
\]
where \( \kappa_{\text{vol}}(\varepsilon_{\text{vol}}^p) \) and \( \kappa_{\text{dev}}(\varepsilon_{\text{dev}}^p) \) are the volumetric and deviatoric hardening functions respectively. The hardening function \( \kappa_{\text{mix}}(\varepsilon_{\text{vol}}^p, \varepsilon_{\text{dev}}^p) \) is for coupled terms, and \( \kappa_0 \) is a constant. The specific form of the hardening functions should be determined from appropriate experimental data. The deviatoric hardening function should be calibrated from shear or torsion mechanical tests, and the volumetric hardening function from experiments where a high hydrostatic stress is imposed, e.g. confined compression.

The volumetric and deviatoric plastic strain rates are defined by the equations,

\[
d\varepsilon_{\text{vol}}^p \equiv d\varepsilon_{\text{kk}}^p, \quad (6.70)
\]

\[
d\varepsilon_{\text{dev}}^p \equiv \sqrt{\frac{2}{3}} \, d\varepsilon': d\varepsilon'. \quad (6.71)
\]

where the increment of plastic strain \( d\varepsilon^p \) is defined in (6.3). For the isotropic pressure dependent yield surface given in (6.68), the volumetric and deviatoric plastic strains are given by

\[
\frac{d\varepsilon_{\text{vol}}^p}{d\varepsilon_{\text{eq}}^p} = \frac{f_y(\sigma)}{f_p(\sigma)} \frac{\alpha^2}{[1 + (\alpha/3)^2]} \frac{p}{f_p(\sigma)}, \quad (6.72)
\]

\[
\frac{d\varepsilon_{\text{dev}}^p}{d\varepsilon_{\text{eq}}^p} = \frac{f_y(\sigma)}{f_p(\sigma)} \frac{1}{[1 + (\alpha/3)^2]} \frac{q}{f_p(\sigma)}. \quad (6.73)
\]
Figure 6.7:  **A)** Plot of the stress strain curves predicted using the CFMD model with linear hardening for four different loading scenarios; shear stress \( i = 5 \), uniaxial, confined, and hydrostatic compression \( i = 1 \). Note the unique yield points and different hardening rates for each of the loading scenarios.  **B)** Plot of the hardening function \( \kappa(\varepsilon_p^\text{vol}, \varepsilon_p^\text{dev}) \) with increasing equivalent plastic strain \( \varepsilon_p^\text{eq} \) (the equivalent plastic strain is defined by the work conjugacy condition (6.4)). The hardening rate increases as the loading transitions from purely deviatoric (shear) loading to purely hydrostatic loading.

The total volumetric and deviatoric plastic strains are determined by integrating the respective increments of plastic strain over each plastic step.

The required hardening rate in (6.9) is given with respect to the equivalent plastic strain. It may be determined with respect to the volumetric and deviatoric plastic strains using the chain rule,

\[
\frac{\partial \kappa(\varepsilon_p^\text{vol}, \varepsilon_p^\text{dev})}{\partial \varepsilon_p^\text{eq}} = \frac{\partial \kappa}{\partial \varepsilon_p^\text{vol}} \frac{\partial \varepsilon_p^\text{vol}}{\partial \varepsilon_p^\text{eq}} + \frac{\partial \kappa}{\partial \varepsilon_p^\text{dev}} \frac{\partial \varepsilon_p^\text{dev}}{\partial \varepsilon_p^\text{eq}} \tag{6.74}
\]

With this, the constitutive law is fully defined. When used in conjunction with the yield function (6.68) it is labelled as the Crushable-Foam with mode-dependent hardening (CFMD) model.
6.4.3.1 Mode-Dependent Linear Hardening

To demonstrate how the CFDH model computes different hardening rates depending on the applied mode of loading, a simple linear hardening model is examined. In this scenario the deviatoric and volumetric hardening functions $\kappa_{\text{dev}}(\varepsilon^p_{\text{dev}})$ and $\kappa_{\text{vol}}(\varepsilon^p_{\text{vol}})$ are linear functions of the deviatoric and volumetric plastic strain respectively, and there is no coupling of the terms, the hardening function (6.69) reduces to,

$$
\kappa(\varepsilon^p_{\text{vol}}, \varepsilon^p_{\text{dev}}) = a_{\text{vol}}\varepsilon^p_{\text{vol}} + a_{\text{dev}}\varepsilon^p_{\text{dev}} + \kappa_0
$$

(6.75)

where $a_{\text{vol}}$ and $a_{\text{dev}}$ are the volumetric and deviatoric linear hardening moduli.

Shear, uniaxial, confined, and hydrostatic loads are simulated using the CF yield function (6.68), assuming associated flow. Elastic properties and initial yield stress are as presented in Section 6.4.1. The hardening moduli are chosen arbitrarily; $a_{\text{vol}} = 30 \text{ MPa}$, and $a_{\text{dev}} = 0 \text{ MPa}$ resulting in perfect plasticity in deviatoric loading, $\kappa_0 = 13.16 \text{ MPa}$.

Figure 6.7A plots the stress-strain curve for each of the four loading cases simulated. Figure 6.7B plots the corresponding simulation in terms of the hardening function $\kappa(\varepsilon^p_{\text{vol}}, \varepsilon^p_{\text{dev}})$ with increasing equivalent plastic strain $\varepsilon_{\text{eq}}^p$. Each of the four loading cases has a unique yield point and hardening response. As intended, the hardening rate increases as the mode of loading transitions from deviatoric to hydrostatic, as illustrated in the plot of hardening of as a function of equivalent plastic strain (as defined in (6.4)) in Figure 6.7B.

6.4.3.2 Phenomenological Hardening

Section 6.4.3.1 demonstrates the concept of a mode-dependent hardening function using a simple linear case. In this section, experimental data is used to define the
required deviatoric and volumetric hardening functions.

Firstly, the yield function is calibrated such that the initial yield strength $\kappa(0,0)$ is calculated by $f_y(\sigma)$ by a) the shear yield stress, and b) the stress at yield in confined compression. This calibration results in the yield function parameter $\alpha = 0.94$. The deviatoric hardening function is calibrated by using the experimental shear stress-strain data to calculate a $\kappa_{\text{dev}}(\varepsilon^P_{\text{dev}})$ function, such that the experimental shear stress-strain data is reproduced by the CFDH model. This can be easily achieved, as there is no volumetric stress/strain in this loading case, $\kappa_{\text{vol}}(\varepsilon^P_{\text{vol}}) = \kappa_{\text{vol}}(0)$ throughout. Calibration of the volumetric hardening function is more challenging, as there is no explicit hydrostatic compression test data available. Instead, data from the confined compression experiments are used to calibrate $\kappa_{\text{vol}}$. A confined compression load consists of both deviatoric and volumetric stress (see Figure 6.6), hence $\kappa_{\text{dev}}$ is active in this loading path. However, as $\kappa_{\text{dev}}$ is calibrated in the previous step, it need not be considered when calibrating $\kappa_{\text{vol}}$. A trial volumetric hardening function is created, based on the confined compression data, and is iterated upon until the plasticity model reproduces the experimental confined compression stress-strain data.

Once the two hardening functions have been calibrated the CFDH model is fully defined. Uniaxial compression, confined compression, and shear loading cases are simulated using the CFDH model with phenomenological hardening, the non-associated flow parameter $\beta = 1.54$, and the elastic constants from Section 6.4.2. Figure 6.8 plots the stress-strain curves for each of the loading cases. As the shear and confined compression data are used to calibrate the hardening function, they accurately predict their respective stress-strain curves. However, the uniaxial response is determined entirely by the CFDH model. Figure 6.8 shows that the uniaxial yield point and post-yield hardening rate are accurately captured. hardening at higher strain is reasonably well predicted, with an error of only 28% at a strain of 0.35
Figure 6.8: Plot of the stress-strain curves computed by the CFDH model with phenomenological hardening, alongside the corresponding experimental data. The model is calibrated using the shear and confined compression data, hence it reproduces their stress-strain behaviour. However the uniaxial behaviour is determined solely by the model which computes an excellent prediction of the post-yield hardening.

(compared to 48% for the CFIH model in Figure 6.5). The ability of the CFDH model to predict the hardening behaviour shown in Figure 6.8 an initial validation of this model. Further multiaxial experiments should be performed in future studies to explore alternative paths in the $q - p$ plane.
6.5 Anisotropic Plasticity

Section 6.4 demonstrates the ability of an isotropic CFMH model to simulate multi-axial inelastic behaviour of trabecular bone. However, it is well known that trabecular bone is an anisotropic material which exhibits directionally dependent moduli and yield strengths (Rice et al., 1988; Cowin and Mehrabadi, 1989; Van Rietbergen et al., 1996). Therefore it is necessary to use an anisotropic constitutive law to model this mechanical behaviour. Microstructure based FE models are commonly used to determine macro-scale stress–strain behaviour under various boundary conditions in each of the three principal directions (Van Rietbergen et al., 1996; Niebur et al., 2000). This in silico experiment allows us to test the same specimen multiple times, something which cannot be done using destructive mechanical tests. Two pressure-dependent anisotropic constitutive laws, which are extensions of the isotropic CFDH model, are used to provide a continuum framework that replicates that plastic behaviour determined from the in silico microstructural FE simulations.

6.5.1 Micro-mechanical finite element analysis

The micro-FE model used in this study is based on a microstructure that has previously been validated for on-axis elastic behaviour (Harrison et al., 2008), and on-axis yielding (Kelly et al., 2013b; Harrison et al., 2013). Figure 6.9A shows the 8 mm cube geometry used for the micro-FE model, which is created from a micro-CT scan of an L6 ovine vertebra taken at a resolution of 72 µm (µCT40, Scanco Medical AG, Basserdorf, Switzerland). A FE mesh, consisting of approximately 270,000 tetrahedral elements, is created from this geometry using Mimics (v14.11 Mimics and v6.0 3matic, Materialise, Leuven, Belgium). The constitutive model used for the trabecular bone tissue is isotropic, linear elastic with \( J^2 \) perfect plasticity (where \( f_y(\sigma) = f_p(\sigma) = q \)). A Young’s modulus \( E^{\text{tissue}} \) of 4.0 GPa, elastic Poisson’s ratio
$\nu_{\text{tissue}}$ of 0.3, and uniaxial yield strength $\sigma_y^{\text{tissue}}$ of 66 MPa are used for the tissue material, (Harrison et al., 2008; Kelly et al., 2013b).

FE simulations are performed using Abaqus (v6.11 DS Simulia) to determine the macro-scale stress-strain response of the micro-FE model to: a) uniaxial compression, b) confined compression, and c) simple shear, in each of the three axes of the cube (noting that the on-axis direction of the vertebrae coincides with the 3-direction). This results in nine unique in silico elastic-plastic mechanical tests on the same specimen. All simulations are displacement driven and the appropriate boundary conditions are used for each loading case (Bevill et al., 2009; Pahr and Zysset, 2008).

The macro scale Cauchy stress–log strain response for uniaxial compression, confined compression, and simple shear loading are plotted in Figures 6.9B–D respectively. As shown in 6.9B, the on-axis 3-direction uniaxial stress-strain curve is similar to an elastic-perfectly plastic response. A lower stiffness and yield stress is computed in the off-axis 1- and 2-directions, but significant strain hardening is observed post-yield. Interestingly, like the experimental data presented in Section 6.4.1, the micro-FE model computes an increased hardening rate in confined compression (Figure 6.9C) compared to the response in uniaxial compression (Figure 6.9B). The strain hardening rate is again a function of the body direction. Finally, the three shear simulations shown in Figure 6.9D also exhibit significant anisotropy in terms of stiffness and yield stress, with significant strain hardening being computed in each test.

As established in Figure 6.9, the mechanical response of the micro-FE model is anisotropic. Assuming that the material is orthotropic linear elastic, the nine required material constants for the elasticity tensor are determined from the micro-FE data in uniaxial compression and tension, and in simple shear. These constants are presented in Table 6.4. Additionally, the 0.2% offset yield strength is calculated
Figure 6.9: 

A) Schematic indicating the location in the L6 vertebra from which the 8 mm cube of ovine trabecular bone is taken from the micro-CT scan (Adapted from Kelly et al. (2013b)).  

B) Plot of the macro-scale Cauchy stress–log strain behaviour in uniaxial compression determined from the micro-FE model. Plots are given for each of the three principal directions, \( \{i, i = 11, 22, 33\} \).  

C) Plot of the macro-scale Cauchy stress–log strain behaviour in confined compression determined from the micro-FE model. Plots are given for the direction in which the load is applied, \( ii = \{11, 22, 33\} \).  

D) Plot of the macro-scale Cauchy stress–log strain behaviour in simple shear in three configurations, \( ij = \{12, 13, 23\} \)
Table 6.4: Orthotropic elastic mechanical properties determined from the micro-FE models: Young’s modulus $E_i$, shear modulus $G_{ij}$, and elastic Poisson’s ratio $\nu_{ij}^e$.

<table>
<thead>
<tr>
<th>$E_1$ (MPa)</th>
<th>$E_2$ (MPa)</th>
<th>$E_3$ (MPa)</th>
<th>$G_{12}$ (MPa)</th>
<th>$G_{13}$ (MPa)</th>
<th>$G_{23}$ (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1,063.3</td>
<td>909.2</td>
<td>1,555.0</td>
<td>274.9</td>
<td>397.2</td>
<td>316.8</td>
</tr>
<tr>
<td>$\nu_{21}^e$</td>
<td>$\nu_{31}^e$</td>
<td>$\nu_{32}^e$</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.226</td>
<td>0.288</td>
<td>0.287</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 6.5: Normal and shear yield strengths determined from the uniaxial compression and simple shear micro-FE simulations.

<table>
<thead>
<tr>
<th>$\sigma_{11}^y$ (MPa)</th>
<th>$\sigma_{22}^y$ (MPa)</th>
<th>$\sigma_{33}^y$ (MPa)</th>
<th>$\sigma_{12}^y$ (MPa)</th>
<th>$\sigma_{13}^y$ (MPa)</th>
<th>$\sigma_{23}^y$ (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>16.74</td>
<td>14.25</td>
<td>25.56</td>
<td>6.49</td>
<td>9.47</td>
<td>7.17</td>
</tr>
</tbody>
</table>

from each of the uniaxial compression and simple shear tests. Table 6.5 presents the normal and shear yield strengths.

Finally, Cauchy stress–plastic log strain curves are calculated using the uniaxial compression and simple shear data. Each of these six curves are then used as hardening functions $\kappa_{ij}(\varepsilon_{ij}^p)$ for $ij = \{11, 22, 33, 12, 13, 23\}$. These hardening functions are later used to define the yield function $X_{H05}$ in Section 6.5.2.2. Figure 6.10A shows the hardening function for the uniaxial data as a function of increasing plastic log strain. A plastic Poisson’s ratio as a function of the axial plastic strain is calculated for each of the three uniaxial compression data sets using,

$$\nu_{ij}^p(\varepsilon_{ij}^p) = -\frac{d\varepsilon_{ij}^p}{d\varepsilon_{ii}^p}$$ (6.76)

where $i$ is the direction of applied load, and $j$ is one of the lateral directions. Figure 6.10B plots the plastic Poisson’s ratio as a function of the axial plastic log strain.
6.5.2 Anisotropic yield surfaces and hardening functions

In this section two published plasticity models are used to model the multiaxial mechanical behaviour determined from the micro-FE models. Firstly, an anisotropic extension of the CF model proposed by Xue and Hutchinson (2004) (XH04 model) is used in conjunction with a standard hardening model based on uniaxial data in one direction. Secondly, a modified version of the XH04 model proposed by Xue et al. (2005) (XH05 model) is used. This model features a normalized yield function where each stress term is normalized by its respective hardening function. Additionally, two methods of computing the plastic strain to be input into the hardening functions are investigated, independent and coupled hardening. Initially an infinitesimal strain formulation (Section 6.2.1) is used for the XH04 and XH05 models. Finally, the large deformation formulation (Section 6.2.2) is implemented for the XH05 model.

For the elastic constitutive response, orthotropic linear elasticity is assumed throughout this section: \( \sigma = C^e : \varepsilon \), where \( C^e \) is the orthotropic elasticity ten-
sor. In Voigt notation,

\[
\begin{bmatrix}
\sigma_{11} \\
\sigma_{22} \\
\sigma_{33} \\
\sigma_{12} \\
\sigma_{13} \\
\sigma_{23}
\end{bmatrix} =
\begin{bmatrix}
1/E_1 & -\nu_{21}/E_2 & -\nu_{31}/E_3 & 0 & 0 & 0 \\
-\nu_{12}/E_1 & 1/E_2 & -\nu_{32}/E_3 & 0 & 0 & 0 \\
-\nu_{13}/E_1 & -\nu_{23}/E_2 & 1/E_3 & 0 & 0 & 0 \\
0 & 0 & 0 & 1/G_{12} & 0 & 0 \\
0 & 0 & 0 & 0 & 1/G_{13} & 0 \\
0 & 0 & 0 & 0 & 0 & 1/G_{23}
\end{bmatrix}^{-1}
\begin{bmatrix}
\varepsilon_{11} \\
\varepsilon_{22} \\
\varepsilon_{33} \\
2\varepsilon_{12} \\
2\varepsilon_{13} \\
2\varepsilon_{23}
\end{bmatrix}
\]  

(6.77)

### 6.5.2.1 Pressure-dependent anisotropic yield

The anisotropic pressure-dependent plasticity constitutive law by Xue and Hutchinson (2004) (XH04) is used to model the data from the micro-FE simulations. The yield function can be considered as either a pressure-dependent extension of the Hill yield criterion (Hill, 1948), or an anisotropic extension of the CF model. It is given as,

\[
f_y(\sigma) = \frac{1}{\sqrt{2}} \left( \alpha_{12}(\sigma_{11} - \sigma_{22})^2 + \alpha_{23}(\sigma_{22} - \sigma_{33})^2 + \alpha_{31}(\sigma_{33} - \sigma_{11})^2 + 6\alpha_{44}\sigma_{12}^2 + 6\alpha_{55}\sigma_{13}^2 + 6\alpha_{66}\sigma_{23}^2 + \alpha_{11}\sigma_{11}^2 + \alpha_{22}\sigma_{22}^2 + \alpha_{33}\sigma_{33}^2 \right)^{1/2},
\]

(6.78)

where \(\alpha_{ij}\) are material parameters which dictate the anisotropy of the yield surface.

The final three terms of (6.78) establish the pressure-dependence of the yield function. Note that (6.78) may easily be collapsed to either the plastically incompressible Hill yield function, or to an isotropic Crushable-Foam type yield function.

**Model calibration:** Firstly, this model uses a uniform hardening function which is based on the uniaxial stress–plastic strain behaviour in the 3-direction. The
hardening function used for the yield criterion (6.2) is given as,

\[ \kappa = \kappa(\varepsilon_{eq}^p) = \kappa_{33}(\varepsilon_{eq}^p) \]  

(6.79)

Associated flow is assumed throughout.

The yield function requires nine parameters for calibration. These parameters are calibrated using yield point data. The data points chosen should reflect a diverse range of multiaxial yield points to accurately represent the multiaxial yield surface. In this section, three different yield functions are calibrated using three different sets of multiaxial yield data.

The ratios of the initial shear stress, to the initial yield stress in the 3-direction are readily defined \( R_{ij} = \kappa(0)/\sigma_{ij}^y \) where \( i \neq j \). The parameters \( \alpha_{44}, \alpha_{55}, \) and \( \alpha_{66} \) are readily obtained from (6.78) using:

\[ \alpha_{44} = R_{12}^2/3, \quad \alpha_{55} = R_{13}^2/3, \quad \text{and} \quad \alpha_{66} = R_{23}^2/3. \]

Now, six \( \alpha \) parameters remain to be calibrated. Next, the three normal yield strength ratios are determined, \( R_{ii} = \kappa(0)/\sigma_{ii}^y \) for \( i = \{1, 2, 3\} \) (note that \( R_{33} = 1 \)). Three methods to approximate the remaining parameters of the yield surface are now outlined.

**Method A:** Yield surface A is computed using three uniaxial yield points and three plastic Poisson’s ratios (the initial plastic Poisson’s ratio, \( \nu_{ij}^p(0) \), is used in this case). Using (6.78) and (6.76), six equations are formulated and can be written in
Figure 6.11: Plot of each of the calibrated XH04 anisotropic yield surfaces, normalized by the uniaxial yield strength in the 3-direction. Note that the uniaxial yield point for each of the yield surfaces A–C are coincident for each axis.

Yield surface A is shown in Figure 6.11.

**Method B:** Yield surface B is determined using three uniaxial yield points, two plastic Poisson’s ratios, and the hydrostatic yield ratio, $H = \sigma_{Hydro}^y / \sigma_{ij}^y$. The hydrostatic yield point is determined using a micro-FE model as outlined in Section

$$\begin{bmatrix} \alpha_{12} \\ \alpha_{23} \\ \alpha_{31} \\ \alpha_{11} \\ \alpha_{22} \\ \alpha_{33} \end{bmatrix} = \begin{bmatrix} 1/R_{11}^2 & 0 & 1/R_{11}^2 & 1/R_{11}^2 & 0 & 0 \\ 1/R_{22}^2 & 1/R_{22}^2 & 0 & 0 & 1/R_{22}^2 & 0 \\ 0 & 1/R_{33}^2 & 1/R_{33}^2 & 0 & 0 & 1/R_{33}^2 \\ 1/\nu_{12}^p R_{11}^2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1/\nu_{32}^p R_{22}^2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1/\nu_{31}^p R_{33}^2 & 0 & 0 & 0 \end{bmatrix}^{-1} \begin{bmatrix} 2 \\ 2 \\ 2 \\ 2 \\ 2 \\ 2 \end{bmatrix}$$

(6.80)
6.5.1. The yield point $\sigma_{\text{hydro}}^y$ is determined using a 0.2\% offset of the pressure stress-volumetric strain curve. Using these six sets of data the $B$ matrix is set up as,

$$B = \begin{bmatrix}
    1/R_{11}^2 & 0 & 1/R_{11}^2 & 1/R_{11}^2 & 0 & 0 \\
    1/R_{22}^2 & 1/R_{22}^2 & 0 & 0 & 1/R_{22}^2 & 0 \\
    0 & 1/R_{33}^2 & 1/R_{33}^2 & 0 & 0 & 1/R_{33}^2 \\
    0 & 0 & 0 & 1/H^2 & 1/H^2 & 1/H^2 \\
    0 & 1/\nu_{32}^p R_{22}^2 & 0 & 0 & 0 & 0 \\
    0 & 0 & 1/\nu_{31}^p R_{33}^2 & 0 & 0 & 0
\end{bmatrix} \quad (6.81)$$

Yield surface B is shown in Figure 6.11.

Method C: Yield surface C is determined using three uniaxial yield points, the hydrostatic yield ratio $H$, and the assumption that the pressure dependent coefficients are equal ($\alpha_{11} = \alpha_{22} = \alpha_{33}$). In this case the $B$ matrix is,

$$B = \begin{bmatrix}
    1/R_{11}^2 & 0 & 1/R_{11}^2 & 1/R_{11}^2 & 0 & 0 \\
    1/R_{22}^2 & 1/R_{22}^2 & 0 & 0 & 1/R_{22}^2 & 0 \\
    0 & 1/R_{33}^2 & 1/R_{33}^2 & 0 & 0 & 1/R_{33}^2 \\
    0 & 0 & 0 & 3/H^2 & 0 & 0 \\
    0 & 0 & 0 & 0 & 3/H^2 & 0 \\
    0 & 0 & 0 & 0 & 0 & 3/H^2
\end{bmatrix} \quad (6.82)$$

Yield surface C is shown in Figure 6.11.

A summary of the material parameters $\alpha_{ij}$ determined for each of the yield surfaces A-C is given in Table 6.6. Once the elasticity tensor, yield function, and hardening function are established, the XH04 constitutive law is fully calibrated. It
Table 6.6: Material parameters calibrated from the micro-E data for the XH04 yield surface (6.78).

<table>
<thead>
<tr>
<th></th>
<th>$\alpha_{12}$</th>
<th>$\alpha_{23}$</th>
<th>$\alpha_{31}$</th>
<th>$\alpha_{11}$</th>
<th>$\alpha_{22}$</th>
<th>$\alpha_{33}$</th>
<th>$\alpha_{44}$</th>
<th>$\alpha_{55}$</th>
<th>$\alpha_{66}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>1.278</td>
<td>0.724</td>
<td>0.760</td>
<td>2.634</td>
<td>4.441</td>
<td>0.516</td>
<td>5.162</td>
<td>2.426</td>
<td>4.237</td>
</tr>
<tr>
<td>B</td>
<td>3.089</td>
<td>0.724</td>
<td>0.760</td>
<td>0.813</td>
<td>2.619</td>
<td>0.516</td>
<td>5.162</td>
<td>2.426</td>
<td>4.237</td>
</tr>
<tr>
<td>C</td>
<td>3.889</td>
<td>1.227</td>
<td>-0.543</td>
<td>1.316</td>
<td>1.316</td>
<td>1.316</td>
<td>5.162</td>
<td>2.426</td>
<td>4.237</td>
</tr>
</tbody>
</table>

is then used to predict post-yield behaviour in uniaxial compression and confined compression.

Figure 6.12A gives the Cauchy stress-log strain response predicted by the XH04 model in uniaxial compression in the three principal directions, alongside the response computed from the micro-FE models. As the hardening function for the model is based on the uniaxial stress-plastic strain data in the 3-direction, the XH04 model accurately predicts the uniaxial response in the 3-direction. As all of the yield surfaces tested are based on the three uniaxial yield points, the XH04 model correctly predicts the yield point in the 1- and 2- directions. However, it cannot accurately model the post-yield hardening correctly in these directions. Each of the yield functions A-C predict the same behaviour in uniaxial compression, as they are all calibrated using the same uniaxial data.

Figure 6.12B gives the axial Cauchy stress-log strain response predicted by the XH04 model in confined compression for each of the three principal directions, and for each of the yield functions A-C. Each of the yield functions accurately predicts the yield point in confined compression. However, the post-yield behaviour is not accurately predicted in any direction. Though the magnitude of the stress post-yield does depend on the specific yield function, all of the fail to exhibit the increased hardening rate observed in the micro-FE tests. The hardening behaviour predicted by the XH04 model in confined compression resembles that seen in uniaxial compression. This is due to limitation that the hardening function is not dependent on
the mode of loading.

Figures 6.12C and D show the normalized yield surfaces, that are defined by the yield functions A-C, in the 2-3 and 1-2 principal stress planes respectively. All of the yield surfaces are similar in the 2-3 plane. It is only in the mechanically weaker 1-2 plane that the differences become apparent.

Though the XH04 model offers great flexibility in predicting the initial yield of a pressure dependent material, it fails to adequately model post-yield behaviour in all loading cases besides that from which the hardening function is derived. Once the yield surface is defined, it is limited to uniform expansion when the material undergoes strain hardening. In the next section, a plasticity model which allows the prescription of loading-mode specific hardening is examined.
Figure 6.12: A) Plot of the Cauchy stress-log strain prediction of the XH04 model in uniaxial compression alongside that computed by the micro-FE model. This model accurately predicts the uniaxial response in the 3-direction. Though the yield point is accurately predicted, the XH04 model fails to predict the post-yield hardening behaviour of the uniaxial tests in the 1- and 2-directions. The same response is computed by each of the yield surfaces A, B, and C. B) Cauchy stress-log strain prediction of the XH04 model in confined compression in the axial direction alongside that computed by the micro-FE model. Each of the three calibrated XH04 yield surfaces are examined, and all of them can predict the yield point in confined compression. However none of the yield surfaces adequately model the post-yield behaviour. C) Normalized plot of the yield surfaces A-C in the 2-3 principal stress plane. D) Normalized plot of the yield surfaces A-C in the 1-2 principal stress plane.
6.5.2.2 Incorporation of loading-mode-dependent, non-uniform hardening model

Section 6.5.2.1 highlights the need for an improved hardening model which incorporates loading mode dependent hardening in order to provide robust and accurate predictions under multiaxial loading. In this section the plasticity model outlined in Xue et al. (2005) (XH05 model) is examined, and its suitability for modelling trabecular bone assessed.

The yield criterion for the XH05 model is defined as,

\[
F = f_y(\sigma, \eta^p) - \sigma_0
\]

which is a variation on the standard yield criterion equation given in (6.2). In the XH05 model a normalized yield function is used, where each component of stress is normalized by its hardening function. Hence the yield function is dependent on both the stress tensor and a plastic strain-type tensor \( \eta^p \). It is defined as,

\[
\left( \frac{f_y(\sigma, \eta^p)}{\sigma_0} \right)^2 = \left( \frac{\sigma_{11}}{\kappa_{11}} \right)^2 + \left( \frac{\sigma_{22}}{\kappa_{22}} \right)^2 + \left( \frac{\sigma_{33}}{\kappa_{33}} \right)^2
\]

\[
+ \left( \frac{\sigma_{12}}{\kappa_{12}} \right)^2 + \left( \frac{\sigma_{13}}{\kappa_{13}} \right)^2 + \left( \frac{\sigma_{23}}{\kappa_{23}} \right)^2
\]

\[
- 2\hat{\nu}_1 \left( \frac{\sigma_{22}\sigma_{33}}{\kappa_{22}\kappa_{33}} \right) - 2\hat{\nu}_2 \left( \frac{\sigma_{11}\sigma_{33}}{\kappa_{11}\kappa_{33}} \right) - 2\hat{\nu}_3 \left( \frac{\sigma_{11}\sigma_{22}}{\kappa_{11}\kappa_{22}} \right)
\]

where \( \hat{\nu}_k \) are functions of the plastic Poisson’s ratios and the hardening functions \( \kappa_{ij} \), which were presented previously in Figure 6.10. The factor \( \sigma_0 \) is a constant reference stress that may be chosen arbitrarily; in this study \( \sigma_0 = \sigma_{33}^y \). Similarly to the XH04 model, the XH05 yield function can be collapsed to either the pressure-independent Hill model or the isotropic CF model by choosing particular values for \( \hat{\nu}_1 \).
In contrast to the XH04 yield function in given in (6.78), the yield function (6.84) is not defined by nine constant material parameters. Instead, it is defined by six hardening functions \( \kappa_{ij}(\eta^p_{ij}) \) for \( ij = \{11, 22, 33, 12, 13, 23\} \) and three plastic Poisson’s ratio functions \( \hat{\nu}_k(\eta^p_{ij}) \) for \( k = \{1, 2, 3\} \), both of which are functions of the plastic strain. Figure 6.10 plots both the hardening functions and the plastic Poisson’s ratio functions determined from the micro-CT tests. As a result of this plastic strain dependence, the evolution of the shape of the yield surface is determined not only by the stress tensor but also by the hardening functions \( \kappa_{ij} \) and the function \( \hat{\nu}_k \). In the simple case where \( \sigma_{ij} \) is the only non-zero component of the stress, the XH05 model uses the corresponding hardening function \( \kappa_{ij} \).

The functions \( \hat{\nu}_k \) are defined by the hardening function and the plastic Poisson’s ratio defined in (6.76), and are given as,

\[
\begin{align*}
\hat{\nu}_1 &= \nu^p_{32} \left( \frac{\kappa_{22}}{\kappa_{33}} \right) = \nu^p_{23} \left( \frac{\kappa_{33}}{\kappa_{22}} \right) \\
\hat{\nu}_2 &= \nu^p_{31} \left( \frac{\kappa_{11}}{\kappa_{33}} \right) = \nu^p_{13} \left( \frac{\kappa_{33}}{\kappa_{11}} \right) \\
\hat{\nu}_3 &= \nu^p_{21} \left( \frac{\kappa_{11}}{\kappa_{22}} \right) = \nu^p_{12} \left( \frac{\kappa_{22}}{\kappa_{11}} \right)
\end{align*}
\]  

(6.85)

As previously stated, as \( \kappa^p_{ij} \) and \( \nu^p_{ij} \) are functions of the plastic strain. Therefore, \( \hat{\nu}_k \) too is a function of the plastic strain.

Two methods are used to determine the plastic strain-type variable \( \eta^p_{ij} \) which is used to drive the evolution of the yield surface with applied load: independent hardening and coupled hardening. Both methods reproduce the corresponding hardening function when there is only one non-zero component of stress. However they produce a different responses in multiaxial stress states.

For the case of independent hardening, the rate of the plastic strain-type variable
is defined using the plastic strain rate as,

\[ d\eta_{ij}^p = |d\varepsilon_{ij}^p| \]  \hspace{1cm} (6.86)

Here, the yield surface evolves according to the magnitude of the plastic strain in a given axis. In other words, hardening in one axis will not result in substantial hardening in any of the other axes, it evolves independently.

For the case of coupled hardening, the rate of the plastic strain-type variable is defined using the equivalent plastic strain rate and the hardening function. It is given as,

\[ d\eta_{ij}^p = (\sigma_0/\kappa_{ij})d\varepsilon_{eq}^p \]  \hspace{1cm} (6.87)

In this case the evolution of the yield surface is coupled to the effective plastic strain, so hardening on one axis will result in hardening on all other axes. However, the magnitude of this coupling effect is scaled through use of the hardening function, \( \kappa_{ij} \), in a specific axis (which is itself a function of \( \eta_{ij}^p \)).

The yield function for the XH05 model is defined using the data determined from the micro-CT models and presented in Section 6.5.1. Associated flow is assumed, and with this the plasticity model is fully defined. Uniaxial compression and confined compression in the three principal directions are simulated using the XH05 model, with both independent and coupled hardening examined.

Figure 6.13A is a plot of the Cauchy stress-log strain curve predicted by the XH05 model in uniaxial compression for both the independent and coupled hardening models. In accordance with (6.84), the XH05 model predicts exactly the uniaxial behaviour computed in the micro-FE models. This is not surprising as this response
has been prescribed; it merely demonstrates that the model is operating as intended.

Figure 6.13B is a plot of the Cauchy stress-log strain curve predicted by the XH05 model in confined compression. The stress-strain response predicted is an improvement on that predicted by the XH04 model (see Figure 6.12). The independent hardening model does not generate substantial hardening in confined compression. Figure 6.13C and 6.13D plot the evolution of the yield surface in its initial state, at an axial strain of $\varepsilon_{33} = 0.125$ for a confined compression in the 3-direction. In the case of independent hardening it is apparent that the yield surface has expanded substantially in the 3-axis, but that little expansion has occurred in the lateral axes. The result of this is that insufficient hardening is generated in the 3-direction, and the confined compression data from the micro-FE models cannot be predicted.

Use of the coupled hardening model results in a further improvement in the prediction of the confined compression behaviour. In this case an increase in the post-yield hardening rate is predicted, as observed in the micro-FE tests. Figures 6.13C and 6.13D demonstrate that the coupled hardening model computes an expansion of the yield surface in all axes. This results in the generation of substantially more hardening in the 3-direction, thereby leading to an improved prediction of the confined compression behaviour.

6.5.2.3 Inclusion of finite deformation plasticity

In this final section, the generic finite deformation plasticity model outlined in Section 6.2.2, together with the XH05 model featuring coupled hardening, is used to model the stress-strain micro-FE data. As outlined in Section 6.3.2, the numerical implementation is reasonably straightforward. The hypoelastic-plastic algorithm used up to now is bookended by a geometric pre-processor and post-processor. The Cauchy stress-log strain micro-FE data used for the hardening functions and orthotropic elasticity tensor must be converted to generalized Kirchhoff stress-log...
Figure 6.13: A) Plot of the Cauchy stress-log strain prediction of the XH05 model in uniaxial compression alongside that computed by the micro-FE model. The hardening function in each direction is based on the uniaxial data, hence the XH05 model computes excellent predictions in all directions. The uniaxial response is the same for both independent and coupled hardening. B) Plot of the Cauchy stress-log strain prediction of the XH05 model in confined compression alongside that computed by the micro-FE model. Results are shown for both independent and coupled hardening. Generally, the coupled hardening model results in a more accurate prediction of the post-yield hardening behaviour. Normalized yield surface for XH05 mode in C) the 2-3 plane, and D) the 1-2 plane. In the initial yield surface is identical for both independent and coupled hardening models. Additionally, the yield surface for a confined compression, $\varepsilon_{33} = 0.125$, using independent and coupled hardening is plotted. Very little hardening occurs in the lateral directions when the independent hardening model is used, whereas significant hardening occurs in all directions with coupled hardening.
Figure 6.14: Plot of the Cauchy stress-log strain response predicted by the XH05FD model and XH05 model with coupled hardening to a confined compression.
strain space. This achieved using (6.29), and can be easily implemented for uniaxial stress in the $i$-direction using $T_i = J\sigma_i$.

Figure 6.14 plots the Cauchy stress-log strain response of the XH05 model including finite deformations (XH05FD model) in confined compression, alongside that computed for the XH05 and in the micro-FE model. Use of the XH05FD model results in a moderate improvement in the prediction of confined compression in each of the three principal directions. In the current study elastic properties are assumed such that the elastic strain at initial yield in the 3-direction is $\sim 1.4\%$. This is rather conservative, with initial yield strains ranging from 1%–3.5% being reported in the literature (Kelly and McGarry, 2012; Rincón-Kohli and Zysset, 2009; Kopperdahl and Keaveny, 1998). In materials that entail high elastic strains at yield, the use of the XH05FD model will be of even greater importance.
6.5.2.4 Modified non-uniform hardening model

A modification to (6.84) is made where one of the plastic Poisson’s ratio terms  \( \hat{\nu}_i \) has been replaced with a term dependent on the hydrostatic stress. This modified yield function (XHM model) is given as,

\[
\left( \frac{f_y(\sigma, \eta^p)}{\sigma_0} \right)^2 = \left( \frac{\sigma_{11}}{\kappa_{11}} \right)^2 + \left( \frac{\sigma_{22}}{\kappa_{22}} \right)^2 + \left( \frac{\sigma_{33}}{\kappa_{33}} \right)^2 + \left( \frac{\sigma_{12}}{\kappa_{12}} \right)^2 + \left( \frac{\sigma_{13}}{\kappa_{13}} \right)^2 + \left( \frac{\sigma_{23}}{\kappa_{23}} \right)^2 - 2\nu^p_{32} \left( \frac{\sigma_{22}\sigma_{33}}{\kappa_{22}^2} \right) - 2\nu^p_{31} \left( \frac{\sigma_{11}\sigma_{33}}{\kappa_{33}^2} \right) + \left( \frac{1}{\phi^2} - \frac{1}{\kappa_{11}^2} - \frac{1}{\kappa_{22}^2} + 2\nu^p_{32} + 2\nu^p_{31} - 1 \right) \sigma_{11}\sigma_{22}
\]

(6.88)

where \( \phi \) is the hydrostatic hardening function which is the hydrostatic stress – volumetric plastic strain response determined from a hydrostatic compression simulation.

The inclusion of the hydrostatic hardening function in this modified yield function means that there is no longer a dependence on data from the uniaxial compression tests to define the multiaxial inelastic behaviour. However (6.88) still retains the elegant property of (6.84) that \( (f_y/\sigma_0) = (\sigma_{ij}/\kappa_{ij}) \) where \( \sigma_{ij} \) is the only non-zero component of stress. In addition, it should be noted that in hydrostatic stress the yield function reduces to \( (f_y/\sigma_0) = (p/\phi) \), where \( p \) is the hydrostatic stress.

This yield function is implemented using coupled hardening and a finite deformation formulation as outlined above. Figure 6.15 plots the stress strain response predicted by the XHM model. Uniaxial compression tests are perfectly predicted, as expected. The inclusion of a hydrostatic stress term in (6.88) results in a substantial improvement in the prediction of the stress-strain behaviour in confined compression.
Figure 6.15: A) Plot of the Cauchy stress-log strain response predicted by the XHM model under uniaxial compression, as expected the uniaxial post-yield behaviour is perfectly predicted. B) Plot of the Cauchy stress-log strain response predicted by the XHM model under confined compression. The inclusion of a hydrostatic term has improved the predictions substantially.
6.6 Discussion

The key findings of the current study on the inelastic behaviour of trabecular bone are as follows:

1. Experimental data shows that trabecular bone features mode-dependent hardening. Its post-yield hardening rate increases as the ratio of deviatoric to pressure stress decreases. This behaviour cannot be captured by current constitutive models (e.g. CFIH model).

2. A novel hardening function is formulated in which the hardening rate changes as a function of the deviatoric and volumetric plastic strain. This hardening together with a Crushable-Foam yield function (CFMD model) can be used to successfully predict multiaxial experimental inelastic data.

3. For the first time, a continuum level anisotropic yield function featuring mode-dependent non-uniform hardening has been used to predict the inelastic behaviour of trabecular bone. It is found that a coupled hardening model leads to the best predictions of multiaxial behaviour, and that the inclusion of finite deformations results in an additional improvement to predictions.

The experimental results of a series of torsion tests on cylindrical specimens of bovine trabecular bone are presented in Section 6.4, alongside previous uniaxial compression and confined compression tests (Kelly and McGarry, 2012). Kelly and McGarry (2012) demonstrate that use of an isotropic CF plasticity model with isotropic hardening can predict the yield point of confined compression data, as well as the uniaxial data from which the model is calibrated. However, in the current paper it is demonstrated that this CFIH model cannot predict the experimental shear behaviour. Additionally, the CFIH model under-predicts the post-yield hardening observed in the confined compression test beyond a strain of 0.1.
Motivated by the observation that as an increase in the ratio of deviatoric stress to pressure stress in trabecular bone leads to an increase in the post-yield hardening rate, a new mode-dependent hardening function is formulated (CFMD model). The hardening behaviour of the material can be tuned using specific deviatoric and volumetric hardening functions. Results for generic linear mode-dependent hardening are presented and, in this case, it is demonstrated that the hardening rate increases as the loading mode becomes more pressure/hydrostatic stress dominant.

The CFMD model, using phenomenological hardening data, can accurately predict post-yield behaviour in confined compression and in shear. Importantly it can also predict the uniaxial behaviour (for which it has not been specifically calibrated). Though there is some error in the uniaxial prediction at higher strains, the CFMD model is a marked improvement on the CFIH model. Some studies have examined the use of pressure-dependent yield surfaces (Garcia et al., 2009; Hosseini et al., 2015), however no previous study has proposed a mode-dependent hardening function. In fact, the topic of post-yield hardening has largely been neglected to date (Mengoni et al., 2012; Garcia et al., 2009).

A number of additional features may be added to the CFMD model to make it more generic. Models for the inclusion of damage in trabecular bone have previously been presented (Charlebois et al., 2010a), and can be incorporated into future CFMD models to predict cyclic behaviour. Furthermore, over-nonlocal damage-plasticity models have been shown to overcome the mesh sensitivity issues encountered in strain softening (Hosseini et al., 2015). The CFMD model can also be modified to include bone morphology/density dependent elasticity tensors and yield functions (Keaveny et al., 2001; Rincón-Kohl and Zysset, 2009; Sanyal and Keaveny, 2013; Zysset, 2003). These features make the model more generic, such that it can be used in continuum whole bone FE simulations where bone tissue is non-homogeneous (e.g. Yosibash et al. (2007)).
In Section 5 the effect of mechanical anisotropy on the multiaxial plastic behaviour of trabecular bone is examined. A micro-mechanical FE model of an 8 mm cube of trabecular bone is used to determine the macro-scale stress-strain behaviour. This method has been successfully applied in previous studies to identify initial yield surfaces of trabecular bone (Bayraktar et al., 2004; Sanyal et al., 2015). An anisotropic pressure-dependent yield function together with a uniform hardening function based on the uniaxial behaviour in the strongest direction (XH04 model) are used to model the stress-strain behaviour determined from the micro-FE models. Three different methods of calibrating the yield surface are presented and results determined using these yield functions are presented.

The XH04 model can only accurately predict the uniaxial data on which the hardening function is based. It fails to satisfactorily predict the uniaxial response in the other two directions. Regardless of which calibrated yield function is used, the XH04 model fails to predict the mechanical behaviour in confined compression. Insufficient hardening is generated by the hardening function, which produces the approximately perfectly-plastic behaviour observed in the 3-direction.

To improve the modelling of post-yield behaviour, the XH05 model is used, which features direction-dependent non-uniform hardening. This model uses hardening functions, which are obtained from phenomenological data, to determine the evolution of the yield surface with applied plastic strain. Two non-uniform hardening models are used to determine the multiaxial hardening response of the XH05 model; independent and coupled hardening.

As prescribed, the XH05 model predicts the uniaxial stress-strain behaviour computed in the micro-FE models. The independent hardening model fails to generate sufficient hardening in confined compression, as significant yield surface expansion occurs only in the direction of applied load. The coupled hardening model does generate an increase in hardening in confined compression, as the yield surface ex-
pands in all axes not just the axis of the applied load. This leads to an improved prediction of the mechanical behaviour in confined compression computed in the micro-FE models. Finally, the incorporation of a finite deformation constitutive framework together with the coupled hardening model (XH05FD model) results in a further moderate improvement in the prediction of the confined compression behaviour. However, the hardening rate predicted by the XH05 and XH05FD is lower than that observed in the micro-FE test.

The remarks made above regarding improvements which can be made to the CFMD model are equally applicable here. The XH04 and XH05 models can incorporate morphological elasticity and yield, in addition to over-nonlocal plasticity and damage. Though studies have examined large deformation plasticity problems for trabecular bone (Hosseini et al., 2015), to the best of the authors knowledge the XH05 model is the first to use a multiplicative split of the deformation gradient. The use of such large deformation plasticity models is important for the for the FE modelling of orthopaedic device implantations (Kelly et al., 2013a,b) and procedures such as balloon kyphoplasty (Purcell et al., 2013).
Bibliography


Concluding Remarks

7.1 Summary of Key Findings

This section summarises the key contributions to the field of biomechanics which have emerged from the research presented in this thesis.

Chapter 3

- It is demonstrated that the compressible HGO-C formulation does not correctly model compressible anisotropic material behaviour. Due to the use of isochoric anisotropic invariants, the anisotropic component of the model is insensitive to volumetric deformation.

- To correctly model compressible anisotropic behaviour a modified anisotropic (MA) model is presented, in which the full anisotropic invariants are used so that a volumetric anisotropic contributions are accounted for. The MA model correctly predicts an anisotropic response in three different case studies hydrostatic tensile loading, pure shear, and uniaxial deformation.

- A finite element user-defined material subroutine is developed for the sim-
ulation of stent deployment in a slightly compressible artery. Significantly higher stress triaxiality and arterial compliance are computed when the full anisotropic invariants are used (MA model) instead of the isochoric form (HGO-C model).

Chapter 4

- In biaxial mechanical testing of cruciform specimens localized unmeasured shear forces occur at the clamps. The inability to quantify such forces has significant implications for the calculation of material stress from simplified force-equilibrium relationships.

- Computational and analytical models of a biaxial tests demonstrate that the unmeasured shear forces arise due to two distinct competing contributions: (1) negative shear force due to stretching of the orthogonal clamp, and (2) positive shear force as a result of material Poisson-effect. The clamp shear force is highly dependent on the specimen geometry and the clamp displacement ratio as, consequently, is the measured force-stress relationship.

- It is demonstrated that commonly accepted formulae for the estimation of material stress in the central region of a cruciform specimen are highly inaccurate. A geometry specific correction factor is proposed for isotropic materials.

- It is demonstrated that a correction factor for the general case of non-linear anisotropic materials is not feasible, and suggest the use of inverse finite element analysis as a practical means of interpreting experimental data for such complex materials.

Chapter 5

- An experimental study of aortic arterial tissue reveals that it is a compressible material. A numerical method is used to determine the bulk and shear moduli
of the tissue ground matrix.

- Biaxial stretch experiments alone are not sufficient to characterise tissue behaviour. It is demonstrated that both an incompressible (HGO) model and a compressible (MA) model can both be accurately calibrated to capture experimental biaxial test data, despite the fact the HGO model neglects material compressibility.

- Failure to accurately characterize tissue compressibility will result in the inaccurate prediction of artery wall material stress in vivo, even if artery compliance is accurately calibrated.

Chapter 6

- Experimental data shows that trabecular bone features mode-dependent hardening. Its post-yield hardening rate increases as the ratio of deviatoric to pressure stress decreases. This behaviour cannot be captured by current constitutive models (e.g. CFIH model).

- A novel hardening function is formulated in which the hardening rate changes as a function of the deviatoric and volumetric plastic strain. This hardening together with a Crushable-Foam yield function (CFMD model) can be used to successfully predict multiaxial experimental inelastic data.

- For the first time, a continuum level anisotropic yield function featuring mode-dependent non-uniform hardening has been used to predict the inelastic behaviour of trabecular bone. It is found that a coupled hardening model leads to the best predictions of multiaxial behaviour, and that the inclusion of finite deformations results in an additional improvement to predictions.
7.2 Future Perspectives

The current thesis has addressed some of the key topics in the field of anisotropic non-linear constitutive modelling of hard and soft tissues. Section 7.1 has summarised the novel contributions of this thesis. These contributions have implications for related topics in biomechanics. The current section discusses these implications and suggests some future studies to address them.

A robust anisotropic hyperelastic constitutive law is presented in Chapter 3. Several studies have incorrectly used the HGO-C constitutive model to simulate; arterial tissue (Cardoso et al., 2014; Iannaccone et al., 2014), cartilage (Peña et al., 2007; Pérez del Palomar and Doblaré, 2006), and the nucleus pulposus (Maquer et al., 2014). The FE simulations in these studies should be re-run using the MA model. The findings in Chapters 3 and 5 determine that when compressibility is correctly implemented, the resultant stress predicted by the MA model is significantly different to that predicted by the HGO-C model. The MA model has the added advantage that it also provides robust solutions for incompressible or slightly incompressible tissue for all boundary conditions, even if the problem is kinematically prescribed and the material is highly confined. Correct prediction of material stress in soft tissue are vital for: a) the design of medical devices (FDA, 2010), b) cell mechanics studies (e.g. Dowling et al. (2012); Reynolds and McGarry (2015)), and c) the design of tissue engineering constructs (Butler et al., 2000; Nerurkar et al., 2007).

The study on arterial compressibility presented in Chapter 5 demonstrated that the ground matrix in arterial tissue is approximately linear. Hence, a neo–Hookean model is used to model the isotropic ground matrix behaviour in the MA model. However, should a non-linear response be observed experimentally, any reasonable isotropic constitutive model with higher order terms or an additional strain invariant,
The relationship between material stress and the force measured in a biaxial test is examined in Chapter 4. It is demonstrated that it is practically impossible to determine the stress in cruciform specimen using only the measured force and standard formulae. This finding has important implications for experimental biomechanics. Biaxial tests are very commonly used to determine the material parameters for constitutive models (Sacks, 2000). Consequently, if the stress-strain curves determined from biaxial tests are incorrect, so too will the material parameters. If this calibrated constitutive law is implemented in a FE simulation, then its results are questionable. For example, this offers a cogent explanation for the ostensibly inconsistent experimental results of Waldman and Lee (2005), where a different stress-strain relationship is reported for a square-like and slender-armed cruciform geometry. An inverse analysis of this data may reveal the “true” material behaviour, which of course is independent of specimen geometry or boundary conditions. It is critical that future biaxial tests implement an inverse FE method based on the force–displacement data to analyse a material.

While Chapter 4 explicitly deals with clamped cruciform specimens, the findings of this chapter also has relevance for square sutured specimens. A preliminary analysis suggests that the force imbalance can be significant at high levels of specimen deformation, even if the rake length is significantly larger than the specimen length (e.g. (Lanir and Fung, 1974)). A more comprehensive study involving FE analysis should be conducted to determine the precise nature of the relationship between the measured force and the material stress in sutured specimens.

In Chapter 5 an experimental study of the compressibility of aortic arterial tissue is presented. Further studies should be conducted on arterial tissue from dif-
ferent anatomical locations to determine their compressibility. The experimental-computational framework established in Chapter 5 offers an robust platform from which to complete this. In addition, measurement of volume change with applied load should be made in future studies. This will allow for the determination of a more precise form of strain energy density for the ground matrix. In addition to using this experiment technique on arterial tissue, it may be applied to different types of tissue. Biaxial tests have been performed on several tissues where incompressibility implicitly assumed (e.g. (Lyons et al., 2014; Shetye et al., 2014)), whereas a full mechanical characterisation should be performed.

Finally, in Chapter 6 constitutive models for the inelastic behaviour of trabecular bone are presented. Future experimental tests on trabecular bone which examine different loading paths in the $p - q$ plane will help to a) more accurately characterise/calibrate the yield surface and the post-yield hardening behaviour. To capture the tension/compression asymmetry for trabecular bone at a macro level (Keaveny et al., 1994), in future micro-FE models a constitutive model which features tension/compression asymmetry should be used for the trabecular bone tissue (Niebur et al., 2000; Schwiedrzik and Zyssset, 2013). A version of the XH05 model which features tension/compression asymmetry should be formulated and calibrated using this data. An additional term may be added to the XH05 yield function which is based on the hydrostatic yield. This will result in a change in shape of the yield surface, which will increase the hardening rate and lead to the more accurate prediction of the confined compression experiments.
Bibliography


Appendix A

Abaqus User Subroutines

A.1 unisohyper_inv

This user subroutine is used to write custom anisotropic hyperelastic constitutive laws. The anisotropy is based on a reinforcing fibre/preferred direction methodology where anisotropic invariants are used to determine anisotropic deformations. The subroutine requires the computation of: the strain energy function $\Psi$, the derivatives of $\Psi$ with respect to each of the invariants, and the second derivatives of $\Psi$ with respect to all combinations of the invariants.

A.1.1 Derivatives of the Modified Anisotropic Hyperelastic Constitutive Law

The expression for the strain energy density is given in the equations below. The important point regarding the MA model is that it uses the total form of the anisotropic hyperelastic invariants. However the unisohyper_inv requires derivatives with respect to the isochoric invariants. This does not limit us to modelling incompressible materials, rather we must form the equations as products of the isochoric invariants.
and the determinant of the deformation gradient, $J$.

\[ \Psi(J, \mathcal{T}_1, \mathcal{T}_4, \mathcal{T}_6) = \Psi_{\text{vol}}(J) + \Psi_{\text{iso}}(\mathcal{T}_1) + \Psi_{\text{aniso}}(J, \mathcal{T}_4, \mathcal{T}_6), \]  

(6.1)

\[ \Psi_{\text{vol}}(J) = \frac{1}{2} \kappa_0 (J - 1)^2, \quad \Psi_{\text{iso}}(\mathcal{T}_1) = \frac{1}{2} \mu_0 (\mathcal{T}_1 - 3), \]  

(6.2)

\[ \Psi_{\text{aniso}}(J, \mathcal{T}_4, \mathcal{T}_6) = \frac{k_1}{2k_2} \sum_{i=4,6} \left\{ \exp\left[ k_2 \left( \frac{J^{2/3}}{\mathcal{T}_i} - 1 \right)^2 \right] - 1 \right\} \]  

(6.3)

The following first derivatives must be computed.

\[ \frac{\partial \Psi}{\partial \mathcal{T}_1} \quad \frac{\partial \Psi}{\partial J} \quad \frac{\partial \Psi}{\partial \mathcal{T}_4} \quad \frac{\partial \Psi}{\partial \mathcal{T}_6} \]

And the following second derivatives must be computed.
Some of the second derivatives are zero and hence are not computed in this algorithm.

A.1.2 MATLAB Code to Compute Strain Energy Derivatives

The MATLAB code below is used to calculate the first and second derivatives of the compressible Modified Anisotropic hyperelastic constitutive law with two families of reinforcing fibres. The variables are named after the required variables in the Fortran code, the index location has been accounted for too. This code uses the Matlab Symbolic Toolbox and computes Fortran-friendly analytical expressions for the derivatives. Some minor changes are required to covert the expressions; for example Matlab uses `^` for an exponent, whereas Fortran uses `**`.

```
clear all; clc

syms BI1 BI2 AJ xkappa xmu xk1 xk2

syms I4bar11 I4bar12 I4bar22 I5bar11 I5bar12 I5bar22

ninv=9;
ainv = sym(zeros(ninv,1));
UI1 = sym(zeros(ninv,1));
```
\texttt{UI2 = sym(zeros(ninv*(ninv+1)/2,1));}

\texttt{%% List of invariants}
\texttt{ainv(1) = BI1;}
\texttt{ainv(2) = BI2;}
\texttt{ainv(3) = AJ;}
\texttt{ainv(4) = I4bar11;}
\texttt{ainv(5) = I5bar11;}
\texttt{ainv(6) = I4bar12;}
\texttt{ainv(7) = I5bar12;}
\texttt{ainv(8) = I4bar22;}
\texttt{ainv(9) = I5bar22;}

\texttt{%% Define the strain energy density}
\texttt{scale = AJ^(2/3);}
\texttt{Uiso = 0.5*xkappa*(AJ-1)^2 + 0.5*xmu*(BI1-3);}
\texttt{Uaniso1 = xk1/(2*xk2)*(exp(xk2*((scale*I4bar11-1)^2))-1);}
\texttt{Uaniso2 = xk1/(2*xk2)*(exp(xk2*((scale*I4bar22-1)^2))-1);}
\texttt{UA = Uiso + Uaniso1 + Uaniso2;}

\texttt{%% First derivatives of U}
\texttt{for i=1:ninv}
\texttt{\hspace{1cm}UI1(i) = simple(diff(UA, ainv(i)));}
\texttt{end}

\texttt{%% Second derivatives of U}
mat = [1 1 1; 4 1 3; 6 3 3; 7 1 4; 9 3 4; 10 4 4; 29 1 8; 31 3 8;...
   32 4 8; 36 8 8];

for c = 1:length(mat)
    UI2(mat(c,1)) = simple(diff(UI1(mat(c,2)),ainv(mat(c,3))));
end